

Building a new DB, current time: 10/26/2018 14:19:06
 New DB name: /Users/ingo/src/protTrace/output/YEAST05874/proteome_YEAST05874
 New DB title: proteome_YEAST05874
 Sequence type: Protein
 Keep MBits: T
 Maximum file size: 1000000000B
 Adding sequences from FASTA; added 6352 sequences in 0.241807 seconds.
 IQ-TREE multicore version 1.6.7.1 for Mac OS X 64-bit built Sep 8 2018
 Developed by Bui Quang Minh, Nguyen Lam Tung, Olga Chernomor,
 Heiko Schmidt, Dominik Schrempf, Michael Woodhams.

Host: Ingos-MBP.local (AVX2, FMA3, 16 GB RAM)
 Command: iqtrees -nt 3 -s ogSeqs_YEAST05874.phy -m WAG -keep-ident -redo
 Seed: 938420 (Using SPRNG - Scalable Parallel Random Number Generator)
 Time: Fri Oct 26 14:19:53 2018
 Kernel: AVX+FMA - 3 threads (4 CPU cores detected)

Reading alignment file ogSeqs_YEAST05874.phy ... Phylip format detected
 Alignment most likely contains protein sequences
 Alignment has 126 sequences with 584 columns, 539 distinct patterns
 379 parsimony-informative, 68 singleton sites, 137 constant sites

	Gap/Ambiguity	Composition	p-value
1	ICHMU 39.38%	failed	0.00%
2	PARTE 39.55%	failed	0.64%
3	PERM5 39.38%	passed	90.25%
4	GIAIB 45.55%	passed	16.23%
5	GIAIC 45.89%	passed	29.42%
6	TUBMM 49.66%	passed	95.99%
7	ASPAC 36.64%	passed	88.19%
8	ASPCL 32.71%	passed	73.70%
9	NEOFI 32.71%	passed	77.74%
10	ASPFN 32.88%	passed	93.23%
11	ASPGI 34.25%	passed	67.17%
12	ASPOR 32.88%	passed	93.23%
13	ASPTN 50.86%	passed	22.91%
14	EMEND 30.99%	passed	93.92%
15	EMENI 30.99%	passed	93.92%
16	ASPFU 32.88%	passed	66.92%
17	PENCH 33.90%	passed	84.53%
18	PENRW 33.90%	passed	84.95%
19	PARBA 34.42%	passed	98.11%
20	DOTSN 34.59%	passed	96.49%
21	PASFU 34.59%	passed	99.00%
22	ZYMTR 43.66%	passed	96.14%
23	AURPU 34.08%	passed	98.51%
24	LEPMJ 35.10%	passed	98.88%
25	PHAND 35.27%	passed	95.59%
26	PHANO 35.27%	passed	95.59%
27	COCLU 34.42%	passed	95.97%
28	BLUGR 34.93%	passed	86.93%
29	SCLS1 34.42%	passed	47.46%
30	COLGR 35.27%	passed	68.30%
31	COLSU 38.01%	passed	76.88%
32	VERDA 42.29%	passed	63.05%
33	VERDV 42.29%	passed	63.05%
34	HYPAI 34.08%	passed	42.96%
35	HYPJE 44.18%	passed	51.07%
36	HYPVG 34.08%	passed	28.37%
37	GIBM7 41.44%	passed	63.40%
38	FUSC1 41.27%	passed	65.16%
39	FUSO4 41.27%	passed	65.16%
40	GIBZA 40.75%	passed	78.06%
41	NECHA 43.15%	passed	37.39%
42	CRYP A 33.73%	passed	83.05%
43	MAGGR 37.67%	passed	52.50%
44	MAGO7 33.22%	passed	76.01%
45	THIHE 31.51%	passed	6.73%
46	NEUCR 31.85%	passed	9.54%
47	NEUT9 32.02%	passed	9.43%
48	PESFW 29.62%	passed	12.93%
49	DEBHA 44.01%	passed	96.30%
50	PICST 44.69%	passed	89.83%
51	CANTE 44.69%	passed	94.63%
52	ASHGO 45.38%	passed	99.74%
53	KAZNA 45.72%	passed	99.34%

54	KLULA	45.21%	passed	98.76%
55	LACTC	44.86%	passed	99.95%
56	CANGA	45.72%	passed	92.34%
57	YEAST	45.55%	passed	99.75%
58	YEASA	45.55%	passed	99.75%
59	YEASO	45.55%	passed	99.75%
60	YEASV	45.55%	passed	99.75%
61	VANPO	45.38%	passed	99.39%
62	ZYGRO	45.38%	passed	99.69%
63	GLOTR	45.03%	passed	28.65%
64	CRYNJ	44.35%	passed	50.01%
65	VAVCU	54.45%	passed	29.98%
66	MUCCI	50.17%	passed	82.25%
67	RHIOR	47.26%	passed	63.54%
68	TURTR	58.90%	passed	92.59%
69	PTEVA	59.93%	passed	68.45%
70	CHOHO	54.45%	passed	82.42%
71	MACEU	60.10%	passed	48.46%
72	TETUR	47.43%	passed	81.04%
73	MEGSC	60.79%	passed	93.37%
74	DROBM	45.55%	passed	99.75%
75	THEKT	59.25%	passed	17.02%
76	CYAME	38.87%	failed	0.45%
77	GALSU	43.66%	passed	31.79%
78	BLAHO	46.23%	passed	65.55%
79	CHLRE	34.08%	failed	0.54%
80	VOLCA	34.25%	failed	3.46%
81	CHLVA	46.58%	passed	5.68%
82	OSTLU	45.21%	passed	87.24%
83	OSTTA	41.10%	passed	81.82%
84	MICCC	44.18%	passed	77.54%
85	KLEFL	40.07%	passed	95.87%
86	PHYPA	31.16%	passed	85.09%
87	MARPO	52.23%	passed	80.00%
88	ORYBR	38.87%	passed	97.57%
89	ORYGL	38.18%	passed	89.91%
90	ORYNI	37.67%	passed	83.35%
91	ORYPU	37.67%	passed	72.83%
92	ORYRU	37.67%	passed	79.77%
93	ORYSI	37.67%	passed	83.35%
94	ORYSJ	37.67%	passed	83.35%
95	BRADI	39.38%	passed	96.46%
96	HORVV	39.04%	passed	93.91%
97	WHEAT	39.04%	passed	96.20%
98	TRIUUA	39.04%	passed	96.20%
99	SORBI	38.53%	passed	97.80%
100	MAIZE	39.38%	passed	98.70%
101	SETIT	38.53%	passed	91.05%
102	MUSAC	45.38%	passed	78.58%
103	MUSAM	45.38%	passed	78.58%
104	CHEQI	37.84%	passed	98.66%
105	NICAT	38.87%	passed	99.33%
106	SOLLC	39.38%	passed	98.98%
107	SOLTU	39.38%	passed	98.67%
108	CUCSA	40.24%	passed	91.28%
109	LUPAN	39.55%	passed	71.85%
110	LOTJA	40.24%	passed	66.07%
111	SOYBN	39.73%	passed	79.37%
112	MEDTR	39.90%	passed	86.44%
113	MANES	40.58%	passed	95.10%
114	POPTR	39.55%	passed	83.67%
115	PRUPE	40.75%	passed	98.48%
116	ARAAL	40.75%	passed	87.76%
117	BRARP	41.44%	passed	96.58%
118	BRANA	41.44%	passed	93.48%
119	BRAOL	45.55%	passed	87.41%
120	ARALY	39.73%	passed	92.00%
121	ARATH	39.55%	passed	93.74%
122	THECC	40.58%	passed	99.37%
123	GOSHI	40.24%	passed	98.97%
124	GOSRA	40.24%	passed	98.82%
125	VITVI	51.37%	passed	80.29%
126	AMBTC	40.58%	passed	99.07%

WARNING: 11 sequences contain more than 50% gaps/ambiguity

**** TOTAL 40.94% 5 sequences failed composition chi2 test (p-value<5%; df=19)

Create initial parsimony tree by phylogenetic likelihood library (PLL)... 0.041 seconds

NOTE: 10 MB RAM (0 GB) is required!
Estimate model parameters (epsilon = 0.100)
1. Initial log-likelihood: -31290.913
Optimal log-likelihood: -30775.795
Parameters optimization took 1 rounds (0.120 sec)
Computing ML distances based on estimated model parameters... 1.384 sec
Computing BIONJ tree...
0.016 seconds
Log-likelihood of BIONJ tree: -30812.792

INITIALIZING CANDIDATE TREE SET

Generating 98 parsimony trees... 3.993 second
Computing log-likelihood of 98 initial trees ... 5.440 seconds
Current best score: -30723.209

Do NNI search on 20 best initial trees
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 1: -30696.728
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 6: -30693.408
Iteration 10 / LogL: -30699.378 / Time: 0h:0m:13s
Iteration 20 / LogL: -30709.821 / Time: 0h:0m:16s
Finish initializing candidate tree set (20)
Current best tree score: -30693.408 / CPU time: 15.871
Number of iterations: 20

OPTIMIZING CANDIDATE TREE SET

Iteration 30 / LogL: -30696.433 / Time: 0h:0m:23s (0h:1m:0s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 34: -30691.848
Iteration 40 / LogL: -30699.641 / Time: 0h:0m:29s (0h:1m:11s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 50: -30691.803
Iteration 50 / LogL: -30691.803 / Time: 0h:0m:35s (0h:1m:12s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 51: -30691.547
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 58: -30691.113
Iteration 60 / LogL: -30696.084 / Time: 0h:0m:41s (0h:1m:9s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 61: -30690.718
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 67: -30690.642
Iteration 70 / LogL: -30691.165 / Time: 0h:0m:47s (0h:1m:7s left)
Iteration 80 / LogL: -30697.402 / Time: 0h:0m:54s (0h:0m:59s left)
Iteration 90 / LogL: -30697.297 / Time: 0h:1m:0s (0h:0m:52s left)
Iteration 100 / LogL: -30691.577 / Time: 0h:1m:6s (0h:0m:44s left)
Iteration 110 / LogL: -30783.542 / Time: 0h:1m:11s (0h:0m:37s left)
Iteration 120 / LogL: -30693.446 / Time: 0h:1m:17s (0h:0m:30s left)
Iteration 130 / LogL: -30810.172 / Time: 0h:1m:23s (0h:0m:24s left)
Iteration 140 / LogL: -30700.696 / Time: 0h:1m:30s (0h:0m:17s left)
Iteration 150 / LogL: -30692.106 / Time: 0h:1m:35s (0h:0m:10s left)
Iteration 160 / LogL: -30694.096 / Time: 0h:1m:42s (0h:0m:4s left)
TREE SEARCH COMPLETED AFTER 168 ITERATIONS / Time: 0h:1m:47s

FINALIZING TREE SEARCH

Performs final model parameters optimization
Estimate model parameters (epsilon = 0.010)
1. Initial log-likelihood: -30690.642
Optimal log-likelihood: -30690.641
Parameters optimization took 1 rounds (0.043 sec)
BEST SCORE FOUND : -30690.641
Total tree length: 18.634

Total number of iterations: 168
CPU time used for tree search: 286.450 sec (0h:4m:46s)
Wall-clock time used for tree search: 106.505 sec (0h:1m:46s)
Total CPU time used: 288.786 sec (0h:4m:48s)
Total wall-clock time used: 107.364 sec (0h:1m:47s)

Analysis results written to:

IQ-TREE report: ogSeqs_YEAST05874.phy.iqtree
Maximum-likelihood tree: ogSeqs_YEAST05874.phy.treefile
Likelihood distances: ogSeqs_YEAST05874.phy.mldist
Screen log file: ogSeqs_YEAST05874.phy.log

Date and Time: Fri Oct 26 14:21:41 2018

rm: temp_parameters_YEAST05874.txt: No such file or directory

Start time: Fri, 26 Oct 2018 14:18:54 +0000

Running for OMA id: YEAST05874

('Prot_id: ', 'YEAST05874')

ogIds_YEAST05874.txt

('#####\tCreating working directory:\n', '/Users/ingo/src/protTrace/output/YEAST05874')

Parsing gene set for species YEAST from OMA database

Making BLAST db of the gene set to be used by the blast search

TIME TAKEN: 0.208922815323 mins Species YEAST gene set preparation#####

OMA ids given..

Searching OMA ortholog group for given OMA id YEAST05874

Searching OMA ortholog sequences for YEAST05874

TIME TAKEN: 0.564103416602 mins Orthologs search in OMA database.

Performing MSA of the orthologs sequences

TIME TAKEN: 0.223083515962 mins MAFFT#####

Tree reconstruction and scaling factor calculation

Reusing existing alignment file: phy_file

Scaling factor: 0.7105030041

TIME TAKEN: 2.53386054834 mins RAxML#####

Transforming MSA based on indel blocks

Calculating indels

('IQ-Tree command: ', '/Users/ingo/anaconda/envs/py27/bin/iqtree -s /Users/ingo/src/protTrace/output/YEAST05874/ogSeqs_YEAST05874.trans /Users/ingo/src/protTrace/output/YEAST05874/ogSeqs_YEAST05874.phy.treefile -tina -st MULTI')

('Indel: ', 0.2202745620559213)

Generating domain constraints for REvolver#####

Preparing XML configuration file for REvolver

Running REvolver / BLAST cycles:

Read 74 items

null device

1

Run: 9
Run: 10
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Run: 13
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Run: 89

TIME TAKEN: 5.7633101662 mins REvolver/BLAST#####

Calculating decay parameters

Decay parameter calculation command: /usr/local/bin/Rscript --quiet --vanilla /Users/ingo/src/protTrace/used_files/r_nonlinear_leastsquare.R decay_summary_YEAST05874.txt

End time: Fri, 26 Oct 2018 14:28:13 +0000

TOTAL TIME: 0.155436160233 hours#####