```
Building a new DB, current time: 10/29/2018 14:32:48
New DB name:   /Users/ingo/src/protTrace/output/human_ZNT3/proteome_human_ZNT3
New DB title:  proteome_human_ZNT3
Sequence type: Protein
Keep MBits: T
Maximum file size: 1000000000B
Adding sequences from FASTA; added 30709 sequences in 0.86847 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-MacBook-Pro.local (AVX2, FMA3, 16 GB RAM)
Command: iqtree -nt 3 -s ogSeqs_human_ZNT3.phy -m WAG -keep-ident -redo
Seed:    632079 (Using SPRNG - Scalable Parallel Random Number Generator)
Time:    Mon Oct 29 14:34:22 2018
Kernel:  AVX+FMA - 3 threads (4 CPU cores detected)

Reading alignment file ogSeqs_human_ZNT3.phy ... Phylip format detected
Alignment most likely contains protein sequences
Alignment has 194 sequences with 1051 columns, 924 distinct patterns
532 parsimony-informative, 246 singleton sites, 273 constant sites
        Gap/Ambiguity  Composition  p-value
    1  ACIFD   70.98%    failed      0.00%
    2  ACIC1   70.88%    failed      0.00%
    3  THEBD   68.32%    failed      0.01%
    4  CATAD   66.98%    failed      0.80%
    5  MYCA9   69.17%    passed     30.23%
    6  MYCIA   71.36%    passed     17.66%
    7  MYCMM   68.70%    failed      1.82%
    8  NOCFA   66.98%    passed      7.89%
    9  SEGRD   68.89%    passed     11.72%
   10  TSUPD   66.98%    failed      0.85%
   11  FRACC   61.47%    failed      0.00%
   12  FRAIE   62.23%    failed      0.00%
   13  FRASN   65.27%    failed      0.00%
   14  FRADG   66.60%    failed      0.00%
   15  ACTS5   67.94%    passed     12.53%
   16  KRIFD   67.55%    failed      1.89%
   17  ACIA4   71.08%    failed      1.32%
   18  CUTAK   71.17%    passed     18.50%
   19  PROAS   71.17%    passed     17.49%
   20  PROFC   69.93%    passed     19.35%
   21  PSEUX   68.32%    failed      1.92%
   22  RUBXD   70.12%    failed      1.36%
   23  KITSK   66.60%    failed      0.05%
   24  STRAW   64.70%    failed      3.96%
   25  STRBB   67.94%    passed     25.35%
   26  STREN   66.41%    failed      0.78%
   27  STRRD   69.84%    failed      1.41%
   28  THECD   68.22%    failed      0.38%
   29  CONWI   69.46%    failed      2.61%
   30  HYDTT   71.27%    failed      4.51%
   31  HYDS0   72.79%    failed      0.00%
   32  BACT6   71.84%    failed      0.14%
   33  PALPW   69.36%    failed      1.13%
   34  CYCMS   71.74%    failed      0.00%
   35  SPILD   70.98%    failed      0.61%
   36  MARTH   71.93%    failed      0.00%
   37  CHLL2   70.79%    passed     38.53%
   38  CHLT3   70.60%    failed      0.31%
   39  DESIS   67.94%    passed     21.66%
   40  DEIPM   70.03%    failed      0.50%
   41  ALIAT   75.26%    passed     35.73%
   42  ALIAD   69.84%    passed     30.49%
   43  BACC1   70.03%    passed      5.60%
   44  BACMQ   70.79%    passed     31.94%
   45  BACMD   70.79%    passed     24.08%
   46  GEOKA   70.03%    failed      0.03%
   47  GEOSW   70.03%    failed      0.03%
   48  GEOS0   70.12%    failed      2.79%
   49  GEOTC   70.12%    failed      2.79%
   50  GEOS4   70.79%    failed      3.53%
   51  PAESJ   67.17%    failed      3.16%
   52  LACAC   71.55%    failed      0.03%
   53  LACCS   71.55%    failed      0.10%
   54  LACDN   71.93%    failed      0.54%
```

55	LACH4	71.55%	failed	0.00%
56	STRGC	72.98%	failed	0.29%
57	STRSV	72.31%	failed	0.03%
58	DESDL	71.17%	passed	13.79%
59	THEPJ	70.03%	passed	7.27%
60	STRM9	70.88%	failed	0.00%
61	IGNAJ	73.64%	failed	0.00%
62	MELRP	71.27%	failed	0.01%
63	THEYD	71.55%	failed	0.00%
64	ASTEC	70.22%	passed	32.35%
65	PHEZH	71.74%	passed	8.31%
66	PARBH	67.75%	passed	33.68%
67	PELHB	70.22%	failed	3.13%
68	METPB	69.74%	failed	0.28%
69	MARAH	73.74%	passed	39.82%
70	SHEFN	69.65%	passed	79.52%
71	PROMH	71.65%	passed	16.61%
72	MARMS	71.74%	passed	32.87%
73	ACIB1	69.74%	failed	1.34%
74	ACIB5	69.74%	failed	2.02%
75	ACIB3	69.74%	failed	2.02%
76	ACIBC	69.74%	failed	1.34%
77	ACIBT	74.88%	failed	0.94%
78	ACIBY	69.74%	failed	2.02%
79	ACIBS	69.74%	failed	2.57%
80	ACIBD	69.74%	failed	2.02%
81	ACICP	69.74%	failed	4.94%
82	PSEAE	71.55%	passed	30.16%
83	PSEA8	71.55%	passed	30.16%
84	PSEA7	71.55%	passed	38.37%
85	PSEAB	71.55%	passed	32.18%
86	PSEFS	71.36%	passed	37.10%
87	PSEF5	71.65%	passed	9.59%
88	PSEPK	71.36%	passed	42.90%
89	PSEP1	71.36%	passed	42.90%
90	PSEPG	71.36%	passed	42.90%
91	PSEPW	71.36%	passed	42.90%
92	PSEU5	70.88%	passed	40.23%
93	PSEUT	79.16%	passed	16.58%
94	LYSEN	71.46%	failed	2.27%
95	PSEUU	65.27%	failed	0.00%
96	STRMK	68.98%	passed	38.59%
97	STRM5	68.98%	passed	16.11%
98	XANAP	67.75%	failed	1.51%
99	XANC8	69.46%	passed	20.68%
100	XANCP	69.46%	passed	20.68%
101	XANCB	69.46%	passed	20.68%
102	XANAC	69.46%	passed	24.69%
103	XANC5	69.46%	passed	23.12%
104	XANOR	68.51%	passed	30.94%
105	XANOM	69.46%	passed	27.89%
106	XANOP	71.08%	passed	16.88%
107	XYLFA	69.46%	passed	9.84%
108	XYLFM	71.46%	passed	16.05%
109	XYLF2	71.46%	passed	16.05%
110	XYLFT	70.79%	passed	20.00%
111	XYLFG	71.46%	passed	16.05%
112	BDEBA	70.50%	passed	21.25%
113	LEPII	69.93%	failed	0.00%
114	VITBC	63.08%	passed	9.74%
115	PERM5	58.33%	failed	3.81%
116	BODSA	55.76%	failed	0.00%
117	EMIHU	60.89%	failed	0.00%
118	MONBE	62.99%	failed	0.00%
119	SPIPN	55.76%	failed	0.44%
120	ENCCU	68.22%	failed	0.00%
121	VAVCU	70.31%	failed	0.00%
122	MUCCI	65.37%	failed	3.28%
123	RHIOR	66.70%	failed	0.42%
124	PHYBL	64.70%	failed	1.82%
125	ORNAN	66.22%	failed	0.17%
126	PROCA	63.37%	failed	0.23%
127	LOXAF	63.75%	failed	0.09%
128	RABIT	61.47%	failed	0.20%
129	OCHPR	66.13%	failed	3.68%
130	DIPOR	66.13%	passed	8.41%

```
131   FUKDA   66.13%   failed   2.11%
132   CAVPO   66.03%   failed   0.36%
133   CHILA   67.75%   failed   4.93%
134   OCTDE   62.80%   failed   0.25%
135   JACJA   63.08%   failed   0.29%
136   MOUSE   67.75%   passed   9.67%
137   RATNO   63.08%   passed   6.23%
138   NANGA   63.08%   failed   1.16%
139   ICTTR   63.08%   failed   0.07%
140   CHLSB   67.75%   failed   4.41%
141   MACMU   63.08%   failed   0.35%
142   PAPAN   63.08%   failed   0.35%
143   GORGO   63.08%   failed   0.11%
144   HUMAN   63.08%   failed   0.11%
145   PANPA   63.75%   failed   0.26%
146   PANTR   63.75%   failed   0.32%
147   PONAB   54.23%   failed   0.00%
148   NOMLE   52.05%   failed   0.00%
149   CALJA   63.18%   failed   0.20%
150   MICMU   66.13%   failed   1.43%
151   OTOGA   63.08%   failed   0.31%
152   TUPBE   66.22%   failed   0.21%
153   CANLF   63.08%   failed   0.15%
154   MUSPF   63.08%   failed   0.21%
155   AILME   63.08%   failed   0.08%
156   FELCA   63.08%   failed   0.01%
157   TURTR   63.08%   failed   0.11%
158   BOVIN   63.08%   failed   0.16%
159   SHEEP   66.13%   failed   0.25%
160   PTEVA   66.13%   failed   0.71%
161   MYOLU   63.65%   failed   1.04%
162   ERIEU   67.65%   failed   4.43%
163   HORSE   66.03%   failed   0.08%
164   DASNO   64.51%   failed   0.00%
165   SARHA   65.94%   passed   14.07%
166   MACEU   63.08%   passed   9.60%
167   ANOCA   63.08%   failed   4.14%
168   BOMMO   59.85%   failed   2.35%
169   DANPL   68.32%   passed   26.74%
170   DENPD   62.23%   failed   0.03%
171   TRICA   63.65%   failed   0.00%
172   DROKI   61.27%   passed   20.01%
173   PEDHC   61.27%   failed   0.00%
174   PHATC   62.42%   failed   1.15%
175   PHYNI   64.32%   failed   3.22%
176   PHYPR   56.80%   failed   2.26%
177   ECTSI   50.24%   failed   0.71%
178   NICAT   64.51%   failed   0.27%
179   SOLLC   64.51%   failed   0.52%
180   SOLTU   63.84%   failed   2.45%
181   CUCSA   63.27%   failed   0.18%
182   LOTJA   59.75%   failed   0.06%
183   SOYBN   62.42%   failed   0.06%
184   MANES   60.70%   failed   0.00%
185   POPTR   64.51%   passed   6.78%
186   PRUPE   63.18%   failed   0.61%
187   ARAAL   66.41%   failed   0.05%
188   BRARP   66.22%   failed   0.21%
189   ARALY   62.23%   failed   0.00%
190   ARATH   64.32%   failed   0.04%
191   THECC   62.13%   failed   3.81%
192   GOSHI   61.08%   failed   0.00%
193   GOSRA   61.66%   failed   0.02%
194   VITVI   65.08%   failed   0.30%
```
WARNING: 194 sequences contain more than 50% gaps/ambiguity
**** TOTAL   67.23% 132 sequences failed composition chi2 test (p-value<5%; df=19)

Create initial parsimony tree by phylogenetic likelihood library (PLL)... 0.104 seconds

NOTE: 28 MB RAM (0 GB) is required!
Estimate model parameters (epsilon = 0.100)
1. Initial log-likelihood: -74299.356
Optimal log-likelihood: -69762.581
Parameters optimization took 1 rounds (0.325 sec)
Computing ML distances based on estimated model parameters... 3.492 sec
Computing BIONJ tree...

```
0.027 seconds
Log-likelihood of BIONJ tree: -69820.055
--------------------------------------------------------------------------
|                   INITIALIZING CANDIDATE TREE SET                       |
--------------------------------------------------------------------------
Generating 98 parsimony trees... 10.404 second
Computing log-likelihood of 98 initial trees ... 12.656 seconds
Current best score: -69709.065

Do NNI search on 20 best initial trees
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 1: -69583.957
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 2: -69579.912
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 3: -69563.775
Iteration 10 / LogL: -69574.906 / Time: 0h:0m:38s
Iteration 20 / LogL: -69593.796 / Time: 0h:0m:54s
Finish initializing candidate tree set (20)
Current best tree score: -69563.775 / CPU time: 51.945
Number of iterations: 20
--------------------------------------------------------------------------
|                   OPTIMIZING CANDIDATE TREE SET                         |
--------------------------------------------------------------------------
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 23: -69551.809
Iteration 30 / LogL: -69561.933 / Time: 0h:1m:13s (0h:3m:54s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 34: -69550.006
Iteration 40 / LogL: -69552.187 / Time: 0h:1m:30s (0h:3m:38s left)
Iteration 50 / LogL: -69582.000 / Time: 0h:1m:50s (0h:3m:8s left)
Iteration 60 / LogL: -69671.889 / Time: 0h:2m:9s (0h:2m:42s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 62: -69549.536
Iteration 70 / LogL: -69572.475 / Time: 0h:2m:30s (0h:3m:19s left)
Iteration 80 / LogL: -69665.735 / Time: 0h:2m:48s (0h:2m:55s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 84: -69546.099
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 85: -69545.131
Iteration 90 / LogL: -69547.836 / Time: 0h:3m:7s (0h:3m:20s left)
Iteration 100 / LogL: -69571.243 / Time: 0h:3m:25s (0h:2m:56s left)
Iteration 110 / LogL: -69563.365 / Time: 0h:3m:45s (0h:2m:34s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 111: -69544.245
Iteration 120 / LogL: -69544.934 / Time: 0h:4m:2s (0h:3m:5s left)
Iteration 130 / LogL: -69554.353 / Time: 0h:4m:21s (0h:2m:43s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 134: -69542.481
Iteration 140 / LogL: -69547.001 / Time: 0h:4m:39s (0h:3m:9s left)
Iteration 150 / LogL: -69559.292 / Time: 0h:4m:58s (0h:2m:48s left)
Estimate model parameters (epsilon = 0.100)
BETTER TREE FOUND at iteration 153: -69542.355
Iteration 160 / LogL: -69548.458 / Time: 0h:5m:15s (0h:3m:4s left)
Iteration 170 / LogL: -69553.564 / Time: 0h:5m:34s (0h:2m:44s left)
Iteration 180 / LogL: -69548.973 / Time: 0h:5m:52s (0h:2m:23s left)
Iteration 190 / LogL: -69583.745 / Time: 0h:6m:9s (0h:2m:3s left)
Iteration 200 / LogL: -69542.864 / Time: 0h:6m:27s (0h:1m:43s left)
Iteration 210 / LogL: -69553.646 / Time: 0h:6m:44s (0h:1m:23s left)
Iteration 220 / LogL: -69548.174 / Time: 0h:7m:3s (0h:1m:3s left)
Iteration 230 / LogL: -69549.416 / Time: 0h:7m:22s (0h:0m:44s left)
Iteration 240 / LogL: -69546.507 / Time: 0h:7m:40s (0h:0m:25s left)
Iteration 250 / LogL: -69576.934 / Time: 0h:7m:58s (0h:0m:5s left)
TREE SEARCH COMPLETED AFTER 254 ITERATIONS / Time: 0h:8m:5s


--------------------------------------------------------------------------
|                     FINALIZING TREE SEARCH                              |
--------------------------------------------------------------------------
Performs final model parameters optimization
Estimate model parameters (epsilon = 0.010)
1. Initial log-likelihood: -69542.355
Optimal log-likelihood: -69542.355
Parameters optimization took 1 rounds (0.102 sec)
BEST SCORE FOUND : -69542.355
Total tree length: 55.023
```

```
Total number of iterations: 254
CPU time used for tree search: 1333.168 sec (0h:22m:13s)
Wall-clock time used for tree search: 483.326 sec (0h:8m:3s)
Total CPU time used: 1339.430 sec (0h:22m:19s)
Total wall-clock time used: 485.539 sec (0h:8m:5s)

Analysis results written to:
  IQ-TREE report:               ogSeqs_human_ZNT3.phy.iqtree
  Maximum-likelihood tree:      ogSeqs_human_ZNT3.phy.treefile
  Likelihood distances:         ogSeqs_human_ZNT3.phy.mldist
  Screen log file:              ogSeqs_human_ZNT3.phy.log

Date and Time: Mon Oct 29 14:42:28 2018
rm: temp_parameters_human_ZNT3.txt: No such file or directory
##### Start time: Mon, 29 Oct 2018 14:32:36 +0000 #####
##### Running for fasta id: human_ZNT3 #####
('Prot_id: ', 'human_ZNT3')
ogIds_human_ZNT3.txt
('#####\tCreating working directory:\n', '/Users/ingo/src/protTrace/output/human_ZNT3')
#####    Parsing gene set for species HUMAN from OMA database        #####
#####    Making BLAST db of the gene set to be used by the blast search       #####
#####    TIME TAKEN: 0.227516651154 mins    Species HUMAN gene set preparation#####
#####    Searching OMA ortholog group for human_ZNT3        #####
#####    Searching OMA ortholog sequences for human_ZNT3     #####
#####    TIME TAKEN: 0.868093649546 mins    Orthologs search in OMA database. #####
#####    Performing MSA of the orthologs sequences #####
#####    TIME TAKEN: 0.679176032543 mins    MAFFT#####
#####    Tree reconstruction and scaling factor calculation #####
Reusing existing alignment file: phy_file
Scaling factor: 1.25391004893
#####    TIME TAKEN: 10.0598454515 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/human_ZNT3/ogSeqs_human_ZNT3.trans /Users/ingo/src/protTrace/output/human_ZNT3/
ogSeqs_human_ZNT3.phy.treefile -tina -st MULTI')
('Indel: ', 0.09028717603523892)
#####    Generating domain constraints for REvolver#####
#####    Preparing XML configuration file for REvolver      #####
##### Running REvolver / BLAST cycles: #####
Read 74 items
null device
          1
Run:  18
Run:  19
Run:  20
Run:  21
Run:  22
Run:  23
Run:  24
Run:  25
Run:  26
Run:  36
Run:  37
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Run:  56
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Run:  58
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Run:  81
Run:  82
Run:  83
Run:  84
Run:  85
Run:  86
```

```
Run:  87
Run:  88
Run:  89
Run:  0
Run:  1
Run:  2
Run:  3
Run:  4
Run:  5
Run:  6
Run:  7
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Run:  64
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Run:  71
Run:  99
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Run:  10
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Run:  75
Run:  76
Run:  77
Run:  78
Run:  79
Run:  80
Run:  90
Run:  91
Run:  92
Run:  93
Run:  94
Run:  95
Run:  96
Run:  97
Run:  98
#####    TIME TAKEN: 13.2023986022 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_human_ZNT3.txt
##### Generating nexus file #####
No likelihood distance found between species: HOMO_SAPIENS and LASALLIA_PUSTULATA. Using
default likelihood distance of 1.0!
Creating matrix file for PhyloProfile...
##### End time: Mon, 29 Oct 2018 14:57:46 +0000 #####
```

TOTAL TIME: 0.419491781924 hours#####