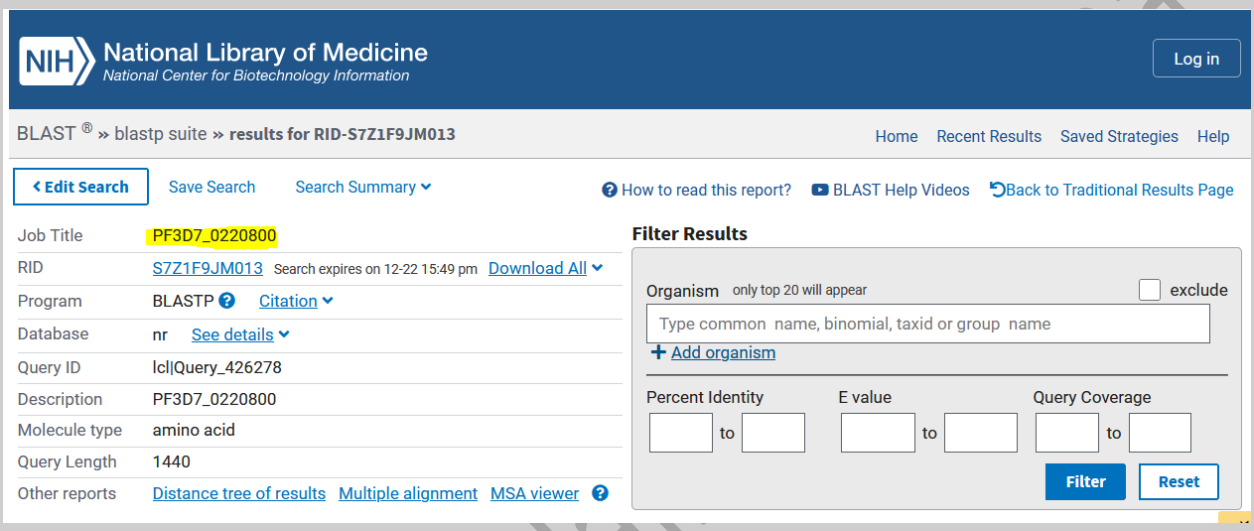
Protein homology modelling using MODELLER

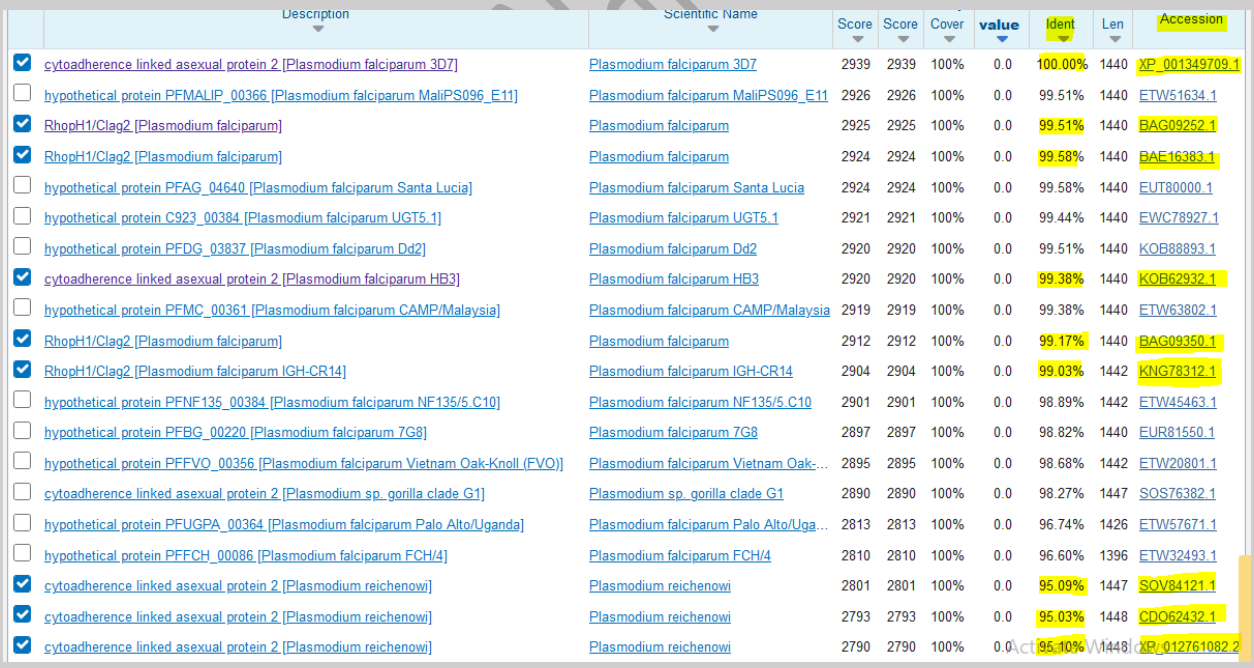
Protein 1: PF3D7_0220800; cytoadherence linked asexual protein 2

Sequence

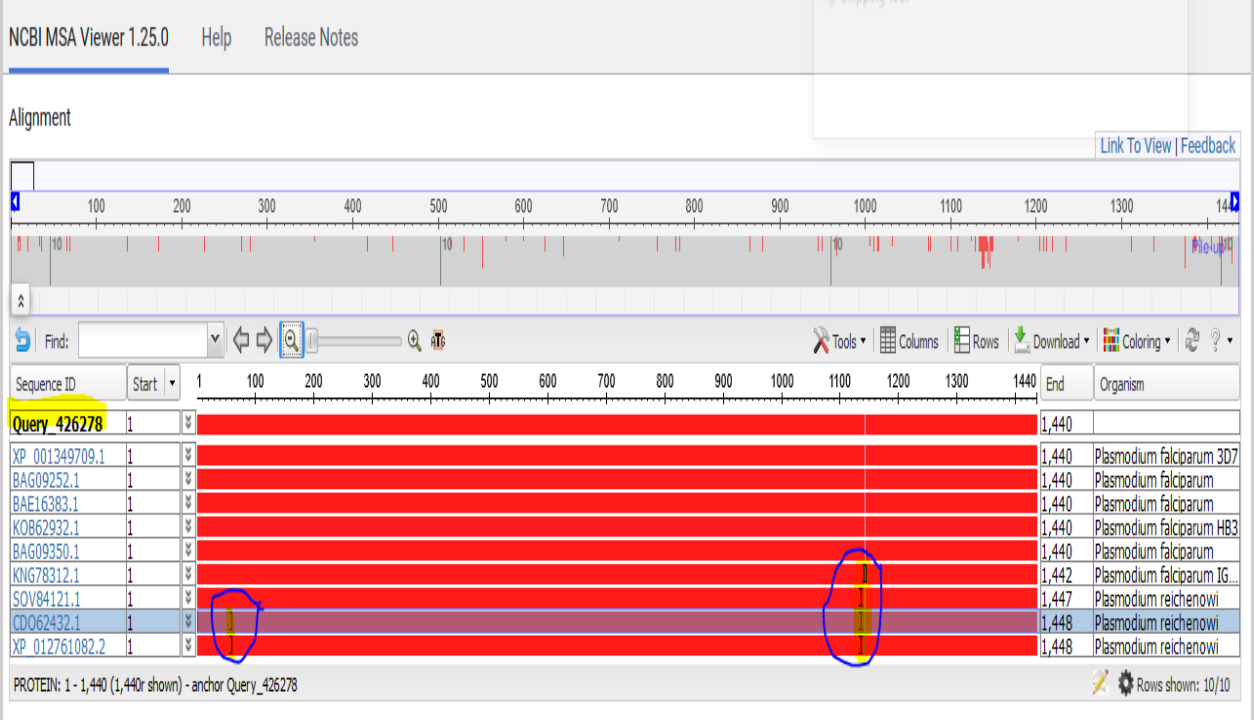
>PF3D7_0220800

https://blast.ncbi.nlm.nih.gov/Blast.cgi#





Description	Scientific Name	Score	Score	Cover	value	Ident	Len	Accession
cytoadherence linked asexual protein 2 [Plasmodium falciparum 3D7]	Plasmodium falciparum 3D7	2939	2939	100%	0.0	100.00%	1440	XP_001349709.1
hypothetical protein PFMALIP_00366 [Plasmodium falciparum MaliPS096_E11]	Plasmodium falciparum MaliPS096_E11	2926	2926	100%	0.0	99.51%	1440	ETW51634.1
RhopH1/Clag2 [Plasmodium falciparum]	Plasmodium falciparum	2925	2925	100%	0.0	99.51%	1440	BAG09252.1
RhopH1/Clag2 [Plasmodium falciparum]	Plasmodium falciparum	2924	2924	100%	0.0	99.58%	1440	BAE16383.1
hypothetical protein PFAG_04640 [Plasmodium falciparum Santa Lucia]	Plasmodium falciparum Santa Lucia	2924	2924	100%	0.0	99.58%	1440	EUT80000.1
hypothetical protein C923_00384 [Plasmodium falciparum UGT5.1]	Plasmodium falciparum UGT5.1	2921	2921	100%	0.0	99.44%	1440	EWC78927.1
hypothetical protein PFDG_03837 [Plasmodium falciparum Dd2]	Plasmodium falciparum Dd2	2920	2920	100%	0.0	99.51%	1440	KOB88893.1
cytoadherence linked asexual protein 2 [Plasmodium falciparum HB3]	Plasmodium falciparum HB3	2920	2920	100%	0.0	99.38%	1440	KOB62932.1
hypothetical protein PFMC_00361 [Plasmodium falciparum CAMP/Malaysia]	Plasmodium falciparum CAMP/Malaysia	2919	2919	100%	0.0	99.38%	1440	ETW63802.1
RhopH1/Clag2 [Plasmodium falciparum]	Plasmodium falciparum	2912	2912	100%	0.0	99.17%	1440	BAG09350.1
RhopH1/Clag2 [Plasmodium falciparum IGH-CR14]	Plasmodium falciparum IGH-CR14	2904	2904	100%	0.0	99.03%	1442	KNG78312.1
hypothetical protein PFNF135_00384 [Plasmodium falciparum NF135/5.C10]	Plasmodium falciparum NF135/5.C10	2901	2901	100%	0.0	98.89%	1442	ETW45463.1
hypothetical protein PFBG_00220 [Plasmodium falciparum 7G8]	Plasmodium falciparum 7G8	2897	2897	100%	0.0	98.82%	1440	EUR81550.1
hypothetical protein PFFVO_00356 [Plasmodium falciparum Vietnam Oak-Knoll (FVO)]	Plasmodium falciparum Vietnam Oak-...	2895	2895	100%	0.0	98.68%	1442	ETW20801.1
cytoadherence linked asexual protein 2 [Plasmodium sp. gorilla clade G1]	Plasmodium sp. gorilla clade G1	2890	2890	100%	0.0	98.27%	1447	SOS76382.1
hypothetical protein PFUGPA_00364 [Plasmodium falciparum Palo Alto/Uganda]	Plasmodium falciparum Palo Alto/Uga...	2813	2813	100%	0.0	96.74%	1426	ETW57671.1
hypothetical protein PFFCH_00086 [Plasmodium falciparum FCH/4]	Plasmodium falciparum FCH/4	2810	2810	100%	0.0	96.60%	1396	ETW32493.1
cytoadherence linked asexual protein 2 [Plasmodium reichenowi]	Plasmodium reichenowi	2801	2801	100%	0.0	95.09%	1447	SOV84121.1
cytoadherence linked asexual protein 2 [Plasmodium reichenowi]	Plasmodium reichenowi	2793	2793	100%	0.0	95.03%	1448	CDO62432.1
cytoadherence linked asexual protein 2 [Plasmodium reichenowi]	Plasmodium reichenowi	2790	2790	100%	0.0	95.10%	1448	XP_012761082.2


NCBI MSA Viewer 1.25.0
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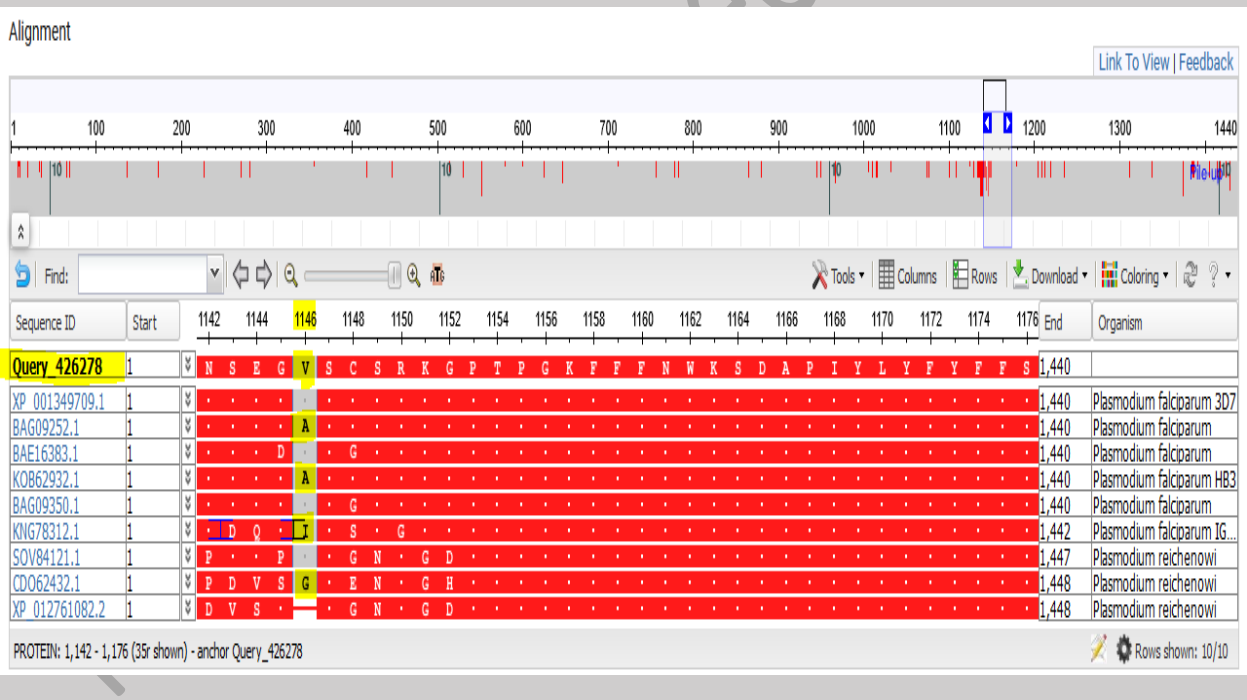
Organism
Query_426278
XP_001349709.1
BAG09252.1
BAE16383.1
KOB62932.1
BAG09350.1
KNG78312.1
SOV84121.1
CDO62432.1
XP_012761082.2
Plasmodium falciparum 3D7
Plasmodium falciparum
Plasmodium falciparum HB3
Plasmodium falciparum IG...
Plasmodium reichenowi
PROTEIN: 1 - 1,440 (1,440r shown) - anchor Query_426278
Rows shown: 10/10


Alignment
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Organism
Query_426278
XP_001349709.1
BAG09252.1
BAE16383.1
KOB62932.1
BAG09350.1
KNG78312.1
SOV84121.1
CDO62432.1
XP_012761082.2
Plasmodium falciparum 3D7
Plasmodium falciparum
Plasmodium falciparum HB3
Plasmodium falciparum IG...
Plasmodium reichenowi
PROTEIN: 1,142 - 1,176 (35r shown) - anchor Query_426278
Rows shown: 10/10

Rows selection

Anchor row Query_426278 cannot be hidden

Name	Sequence ID	Organism	Date	Country	Host	Source	Gene	Identity	Coverage	Mismatches
cytoadherence linked asexual protein 2 [...	XP_001349709.1	Plasmodium falciparum 3D7					PF3D...	100	100	0
RhopH1/Clag2 [Plasmodium falciparum]	BAG09252.1	Plasmodium falciparum (ma...		Honduras				99.51	100	7
RhopH1/Clag2 [Plasmodium falciparum]	BAE16383.1	Plasmodium falciparum (ma...						99.58	100	6
cytoadherence linked asexual protein 2 [...	KOB62932.1	Plasmodium falciparum HB3						99.38	100	9
RhopH1/Clag2 [Plasmodium falciparum]	BAG09350.1	Plasmodium falciparum (ma...		Brazil				99.17	100	12
RhopH1/Clag2 [Plasmodium falciparum IG...	KNG78312.1	Plasmodium falciparum IGH...						99.03	100	12
cytoadherence linked asexual protein 2 [...	SOV84121.1	Plasmodium reichenowi						95.09	100	64
cytoadherence linked asexual protein 2 [...	CDO62432.1	Plasmodium reichenowi						95.03	100	64
cytoadherence linked asexual protein 2 [...	XP_012761082.2	Plasmodium reichenowi	13-Feb-2...	Cameroo...	Pan trogl...	peripher...	PRSY...	95.1	99.93	61

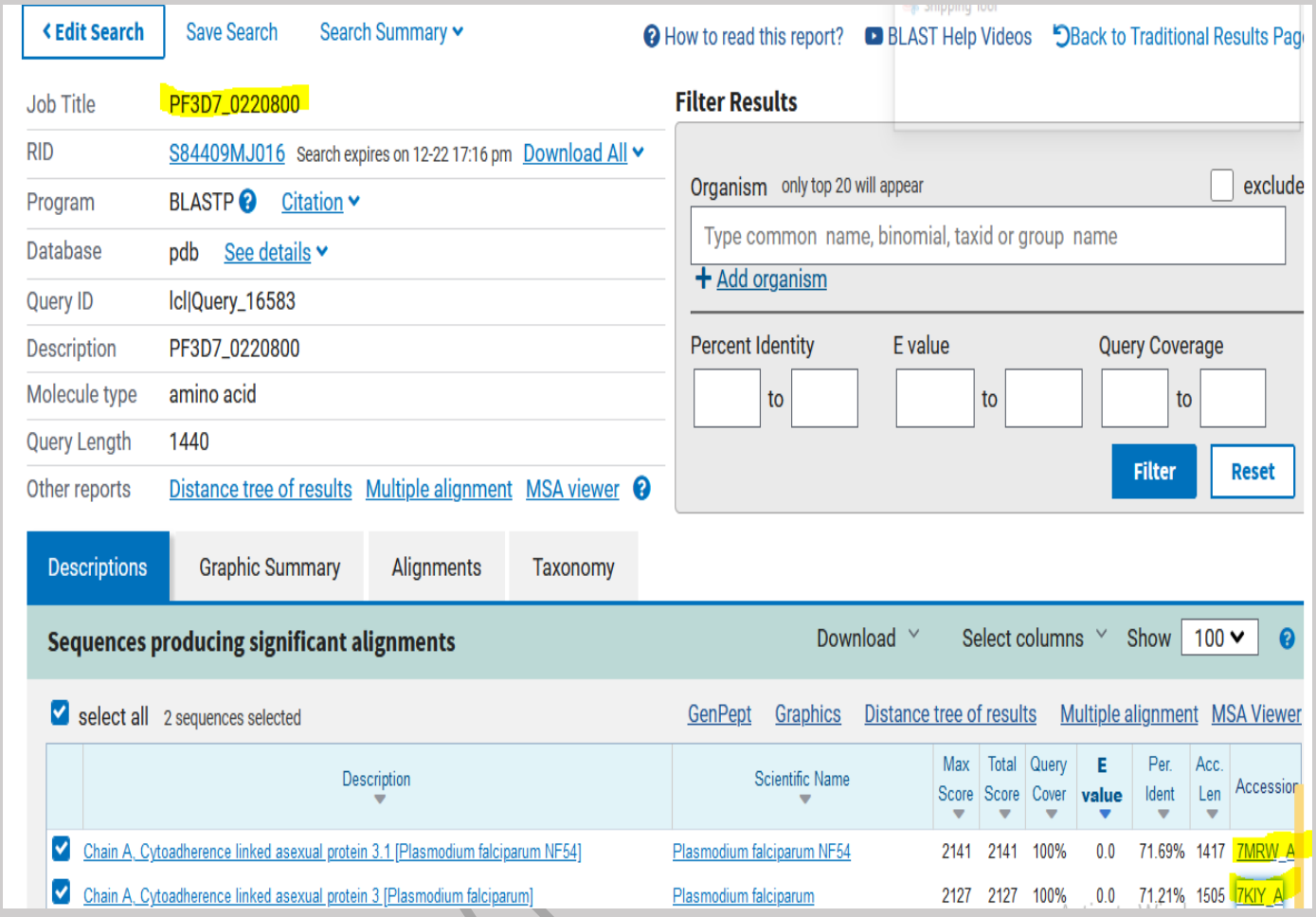
Protein 1: PF3D7_0220800; cytoadherence linked asexual protein 2

SequenceProtein 1: PF3D7_0220800; cytoadherence linked asexual protein 2

Sequence

>PF3D7_0220800

MVSSVKSSLFLLIFFLYLKKNVICSINDNVNENITEGLDEYEFGNENINESITENVNVNVTENEKDNLIYNDDNNNIEEL
KSMIGNDELHKNLSILEKLILDSLKKDKLKLPLIKEGTEEYLDISKFKKKILTDSDDKTYILPTLESSFYDITKYEHILKEQLIE
EYNSKISDAVKKKLLIVRTLKTIKLMLIPLNAYKEKNDLKIALEELNNVITHRTYETLKKSPIENPGEFFRKLLTHVKEVKE
SKEIENKGEYLILGNDKIEIMDAHDFFFTTNSNIKFMETLDSISNQYGLGLINDLGPHLIALGHFMVLKLALKNYKNYF
EAKNTKFFSWQKILEFSLTDRFKILDMMCDHDVVYYSQDKRRKTYLNVDTSGSSMECNILEFLIHYFNKYQLEIIKAT
QDTDFELHGMMEHKNIKDYFFSFMCNDPKECIIYHTNQFKKEAKEENTFPEEPNREISAYNLYLNYYYFMKRYSSYG
IKKTLYVHLLNLTGLLNYDTRSYVTSLYLPGYYNVVEMSFTEDVEFTTLFNNLLKCIKKCHKEETNTNTSLMDSNSSHN
YFLHEITKCDLCKGAFLYSNMKFEEVPSMLQKFYIYLTEGLRIQKVSFLMKTLDIYQDYSNFLSHDINWYTFLFLFRLTS
FEEISKKSVGEAMYLNIQDEDSFHKTITTNYWFPSPIKKYYTLYVRKHLPNNLLDELEKLMKSSTLEKMKKSINFLVHV
NSFLQLDFFHQLNEPPVGLPRSYPLSLILEHKFKEWMNSSPAGFYFSNYHNPYIRKELHRKVLTEKFEPPKMNKWNE
VLKSLIECAYDMYFEQRHVKNLYKNHNIYNINNKIMLMRDSVDLYKKNFKDVIFFADIFNLRKYLTATPLIKKTWDR
MYYFIYRNTGNSVNFYKYGIIYGFKINKVYLKEVVDELYSIYNFNTDIFSDTSFLQTVYLLFRKIEDSYRTHRRNDHIGV
NNIFFMNVANNYSKLNNEEREMEIHNSMASRYYSKTMFAAFQMLFSTMLSNDANNLDKVYGKSSNIQVATSTTA
FLTFAYVYNGSIMDSLTNRLLPPYAKKPITQLKYGKTFVFSNYFMLASQIYEMLNYKNLSLLCEYQAVASANYYSAKK
LGQFVGRKYFPLTTYYLSLRIRASYGWVHGTETKICNSEGVSCSRKGPTPGKFFFNWKSDAPIYLYFYFFSNLYLDSAK
YFPGGFSTSLKEQTEHVSQKGFKKKPMVHELTKNLILDVTNGFMYAFCFYSIMPLYAYFENVNFYIISNFRFLDRYYN
AFNKYFINFFKTKLKKYTTDVFIKYEYDAYTSMKKYGYLNEVIGSRLSSKNRIVKYIYDSNDDIMNNLRRYDMENRFR
NKMSTYVDEYAFFDDCGKNEVFLNDRCDYCPIVEDLCEPDTKEYQPHTSNIQKVTDKNTTYINYEKLHEESYSQETQ
SDNTDDEKDNDLPDTELMITRLQ



7MRW_A = 71.69% = reference_proteinA = https://www.rcsb.org/structure/7MRW

7KIY_A = 71.22% = reference_proteinB = https://www.rcsb.org/structure/7KIY

= ###### = reference_proteinC

We need reference proteins, which is why we used BLASTP

Scripts

For using Modeller, we need 6 scripts

https://salilab.org/modeller/tutorial/basic.html

1) main_protein.ali
2) build_profile.py
3) compare.py
4) align2d.py
5) model-single.py
6) evaluate_model.py (optional)

main_protein.ali

>P1; main_protein

sequence: main_protein:::::::0.00: 0.00

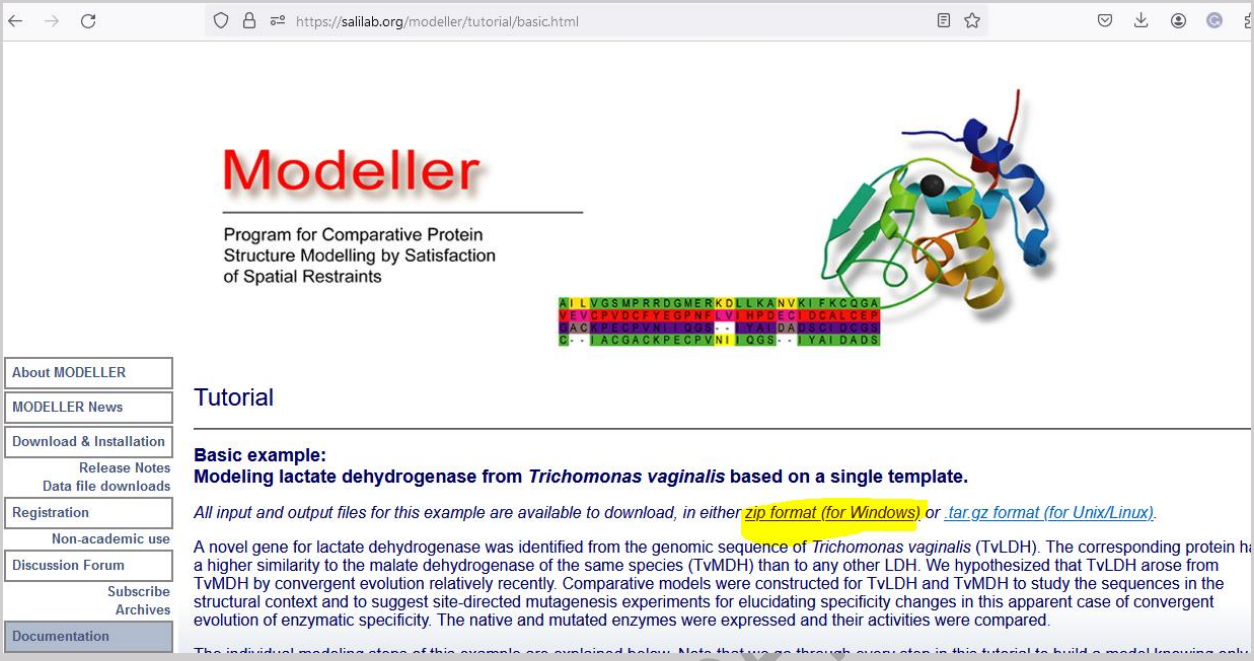
MVSSVKSSLFLLIFFLYLKKNVICSINDNVNENITEGLDEYEFGNENINESITENVNVNVTENEKDNLIYNDDNNNIEEL
KSMIGNDELHKNLSILEKLILDSLKKDKLKLPLIKEGTEEYLDISKFKKKILTDSDDKTYILPTLESSFYDITKYEHILKEQLIE
EYNSKISDAVKKKLLIVRTLKTIKLMLIPLNAYKEKNDLKIALEELNNVITHRTYETLKKSPIENPGEFFRKLLTHVKEVKE
SKEIENKGEYLILGNDKIEIMDAHDFFFTTNSNIKFMETLDSISNQYGLGLINDLGPHLIALGHFMVLKLALKNYKNYF
EAKNTKFFSWQKILEFSLTDRFKILDMMCDHDVVYYSQDKRRKTYLNVDTSGSSMECNILEFLIHYFNKYQLEIIKAT
QDTDFELHGMMEHKNIKDYFFSFMCNDPKECIIYHTNQFKKEAKEENTFPEEPNREISAYNLYLNYYYFMKRYSSYG
IKKTLYVHLLNLTGLLNYDTRSYVTSLYLPGYYNVVEMSFTEDVEFTTLFNNLLKCIKKCHKEETNTNTSLMDSNSSHN
YFLHEITKCDLCKGAFLYSNMKFEEVPSMLQKFYIYLTEGLRIQKVSFLMKTLDIYQDYSNFLSHDINWYTFLFLFRLTS
FEEISKKSVGEAMYLNIQDEDSFHKTITTNYWFPSPIKKYYTLYVRKHLPNNLLDELEKLMKSSTLEKMKKSINFLVHV
NSFLQLDFFHQLNEPPVGLPRSYPLSLILEHKFKEWMNSSPAGFYFSNYHNPYIRKELHRKVLTEKFEPPKMNKWNE
VLKSLIECAYDMYFEQRHVKNLYKNHNIYNINNKIMLMRDSVDLYKKNFKDVIFFADIFNLRKYLTATPLIKKTWDR
MYYFIYRNTGNSVNFYKYGIIYGFKINKVYLKEVVDELYSIYNFNTDIFSDTSFLQTVYLLFRKIEDSYRTHRRNDHIGV
NNIFFMNVANNYSKLNNEEREMEIHNSMASRYYSKTMFAAFQMLFSTMLSNDANNLDKVYGKSSNIQVATSTTA
FLTFAYVYNGSIMDSLTNRLLPPYAKKPITQLKYGKTFVFSNYFMLASQIYEMLNYKNLSLLCEYQAVASANYYSAKK
LGQFVGRKYFPLTTYYLSLRIRASYGWVHGTETKICNSEGVSCSRKGPTPGKFFFNWKSDAPIYLYFYFFSNLYLDSAK
YFPGGFSTSLKEQTEHVSQKGFKKKPMVHELTKNLILDVTNGFMYAFCFYSIMPLYAYFENVNFYIISNFRFLDRYYN
AFNKYFINFFKTKLKKYTTDVFIKYEYDAYTSMKKYGYLNEVIGSRLSSKNRIVKYIYDSNDDIMNNLRRYDMENRFR
NKMSTYVDEYAFFDDCGKNEVFLNDRCDYCPIVEDLCEPDTKEYQPHTSNIQKVTDKNTTYINYEKLHEESYSQETQ

SDNTDDEKDNDLPDTELMITRLQ*

2) build_profile.py

```
from modeller import *

log.verbose()
env = Environ()

#-- Prepare the input files

#-- Read in the sequence database
sdb = SequenceDB(env)
sdb.read(seq_database_file='pdb_95.pir', seq_database_format='PIR',
         chains_list='ALL', minmax_db_seq_len=(30, 4000),
clean_sequences=True)

#-- Write the sequence database in binary form
sdb.write(seq_database_file='pdb_95.bin', seq_database_format='BINARY',
          chains_list='ALL')

#-- Now, read in the binary database
sdb.read(seq_database_file='pdb_95.bin', seq_database_format='BINARY',
         chains_list='ALL')

#-- Read in the target sequence/alignment
aln = Alignment(env)
aln.append(file='main_protein.ali', alignment_format='PIR',
align_codes='ALL')

#-- Convert the input sequence/alignment into
#   profile format
prf = aln.to_profile()

#-- Scan sequence database to pick up homologous sequences
prf.build(sdb, matrix_offset=-450, rr_file='${LIB}/blosum62.sim.mat',
          gap_penalties_1d=(-500, -50), n_prof_iterations=1,
          check_profile=False, max_aln_evalue=0.01)

#-- Write out the profile in text format
prf.write(file='build_profile.prf', profile_format='TEXT')

#-- Convert the profile back to alignment format
aln = prf.to_alignment()

#-- Write out the alignment file
aln.write(file='build_profile.ali', alignment_format='PIR')
```

For pdb_95.bin >>



3_compare.py

```
from modeller import *

env = Environ()
aln = Alignment(env)
for (pdb, chain) in (('reference_protein1_id', 'A'),
('reference_protein2_id', 'A'), ('reference_protein3_id', 'A')):
    m = Model(env, file=pdb, model_segment=('FIRST:'+chain, 'LAST:'+chain))
    aln.append_model(m, atom_files=pdb, align_codes=pdb+chain)
aln.malign()
aln.malign3d()
aln.compare_structures()
aln.id_table(matrix_file='family.mat')
env.dendrogram(matrix_file='family.mat', cluster_cut=-1.0)
```

In compare.log file

```
Sequence identity comparison (ID_TABLE):

   Diagonal       ... number of residues;
   Upper triangle ... number of identical residues;
   Lower triangle ... % sequence identity, id/min(length).

         1b8pA @11bdmA @11civA @25mdhA @27mdhA @21smkA @2
1b8pA @1      327     194     147     151     153      49
1bdmA @1       61     318     152     167     155      56
```

```
1civA @2        45      48     374     139     304      53
5mdhA @2        46      53      42     333     139      57
7mdhA @2        47      49      87      42     351      48
1smkA @2        16      18      17      18      15     313


Weighted pair-group average clustering based on a distance matrix:


                                                .---------------------- 1b8pA
@1.9    39.0000
                                                |
                                        .-------------------------------- 1bdmA
@1.8    50.5000
                                        |
                                    .-------------------------------------- 5mdhA
@2.4    55.3750
                                    |
                                    |                               .--- 1civA
@2.8    13.0000
                                    |                               |
        .-------------------------------------------------------------- 7mdhA
@2.4    83.2500
        |
      .---------------------------------------------------------------- 1smkA
@2.5

      +----+----+----+----+----+----+----+----+----+----+----+----+
    86.0600   73.4150   60.7700   48.1250   35.4800   22.8350   10.1900
         79.7375   67.0925   54.4475   41.8025   29.1575   16.5125
```

4_align2d.py

```
from modeller import *

env = Environ()
aln = Alignment(env)
mdl = Model(env, file='best_model_id', model_segment=('FIRST:A','LAST:A'))
aln.append_model(mdl, align_codes='best_model_id',
atom_files='best_model_id'.pdb')
aln.append(file='main_protein.ali', align_codes='main_protein')
aln.align2d(max_gap_length=50)
aln.write(file='main_protein-best_model_id.ali', alignment_format='PIR')
aln.write(file='main_protein-best_protein_id.pap', alignment_format='PAP')
```

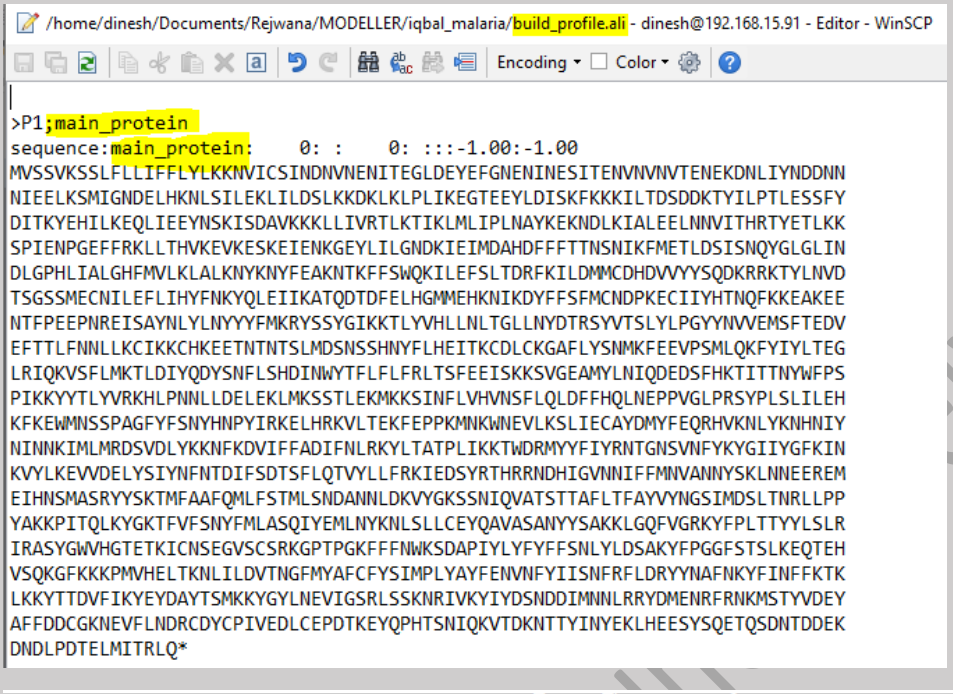
5_model_single.py

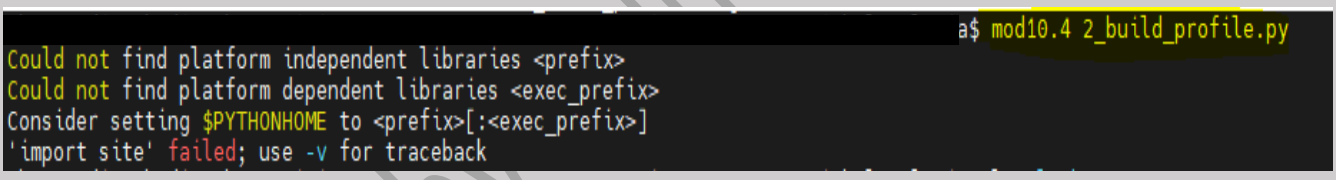
```
from modeller import *
from modeller.automodel import *
#from modeller import soap_protein_od

env = Environ()
a = AutoModel(env, alnfile='main_protein-best_model_id.ali',
```

```
                knowns='best_model_idA', sequence='main_protein',
                assess_methods=(assess.DOPE,
                                #soap_protein_od.Scorer(),
                                assess.GA341))
a.starting_model = 1
a.ending_model = 5
a.make()
```

commands:

2) mod10.4 2_build_profile.py





Note:

#Here, mod10.4 is the version of modeler, it can be different based on the different version of modeler.

#reference protein name and scripts must be same

main_protein.ali

main_protein

main_protein 12/21/2023 6:32 PM ALI File 2 KB

main_protein - Notepad

File Edit Format View Help

```
>P1; main_protein
sequence: main_protein:::::::0.00: 0.00
MVSSVKSSLFLLIFFLYLKKNVICSINDNVNENITEGLDEYEFGNENINESITENVNVNVTENEKDNLIYNDDNNNIEEL
KSMIGNDELHKNLSILEKLILDSLKKDKLKLPLIKEGTEEYLDISKFKKKILTDSDDKTYILPTLESSFYDITKYEHILKEQLIE
EYNSKISDAVKKKLLIVRTLKTIKLMLIPLNAYKEKNDLKIALEELNNVITHRTYETLKKSPIENPGEFFRKLLTHVKEVKE
SKEIENKGEYLILGNDKIEIMDAHDFFFTTNSNIKFMETLDSISNQYGLGLINDLGPHLIALGHFMVLKLALKNYKNYF
EAKNTKFFSWQKILEFSLTDRFKILDMMCDHDVVYYSQDKRRKTYLNVDTSGSSMECNILEFLIHYFNKYQLEIIKAT
QDTDFELHGMMEHKNIKDYFFSFMCNDPKECIIYHTNQFKKEAKEENTFPEEPNREISAYNLYLNYYYFMKRYSSYG
IKKTLYVHLLNLTGLLNYDTRSYVTSLYLPGYYNVVEMSFTEDVEFTTLFNNLLKCIKKCHKEETNTNTSLMDSNSSHN
YFLHEITKCDLCKGAFLYSNMKFEEVPSMLQKFYIYLTEGLRIQKVSFLMKTLDIYQDYSNFLSHDINWYTFLFLFRLTS
FEEISKKSVGEAMYLNIQDEDSFHKTITTNYWFPSPIKKYYTLYVRKHLPNNLLDELEKLMKSSTLEKMKKSINFLVHV
NSFLQLDFFHQLNEPPVGLPRSYPLSLILEHKFKEWMNSSPAGFYFSNYHNPYIRKELHRKVLTEKFEPPKMNKWNE
```

3) mod10.4 3_compare.py

/home/dinesh/Documents/Rejwana/MODELLER/i[redacted]/3_compare.py - [redacted]

Encoding Color

```
from modeller import *

env = Environ()
aln = Alignment(env)
for (pdb, chain) in (('7mrw', 'A'), ('7kiy', 'A'), ('AF-O96279-F1-model_v4', 'A')):
    m = Model(env, file=pdb, model_segment=('FIRST:'+chain, 'LAST:'+chain))
    aln.append_model(m, atom_files=pdb, align_codes=pdb+chain)
aln.malign()
aln.malign3d()
aln.compare_structures()
aln.id_table(matrix_file='family.mat')
env.dendrogram(matrix_file='family.mat', cluster_cut=-1.0)
```

```
(base) [redacted] $ mod10.4 3_compare.py
Could not find platform independent libraries <prefix>
Could not find platform dependent libraries <exec_prefix>
Consider setting $PYTHONHOME to <prefix>[:<exec_prefix>]
'import site' failed; use -v for traceback
```

Note: minimum 3 PDBs are required. Otherwise phylogenetic tree may not generate.

Check 3_compare.log

```
         7mrwA @37kiyA @2AF-O96@1
7mrwA @3     1209    1013     856
7kiyA @2       87    1169     892
AF-O96@1       71      76    1440


Weighted pair-group average clustering based on a distance matrix:


                                                          .--- 7mrwA @3.7    13.0000
                                                          |
       .------------------------------------------------------ 7kiyA @2.9    26.5000
       |
     .------------------------------------------------------- AF-O96@1.0

     +----+----+----+----+----+----+----+----+----+----+----+----+
   27.0400   24.6100   22.1800   19.7500   17.3200   14.8900   12.4600
        25.8250   23.3950   20.9650   18.5350   16.1050   13.6750
```

Here, 7kiyA is the best template model because of low(est) crystallographic resolution (2.9A) & highest similarity (26.5%)

4) mod10.4 4_align2d.py

/home/dinesh/Documents/Rejwana/MODELLER/[redacted]a/4_align2d.py - [redacted]

Encoding ▾ Color ▾

```
from modeller import *

env = Environ()
aln = Alignment(env)
mdl = Model(env, file='7kiy', model_segment=('FIRST:A','LAST:A'))
aln.append_model(mdl, align_codes='7kiyA', atom_files='7kiy.pdb')
aln.append(file='main_protein.ali', align_codes='main_protein')
aln.align2d(max_gap_length=50)
aln.write(file='main_protein-7kiy.ali', alignment_format='PIR')
aln.write(file='main_protein-7kiy.pap', alignment_format='PAP')
```

```
$ mod10.4 4_align2d.py
Could not find platform independent libraries <prefix>
Could not find platform dependent libraries <exec_prefix>
Consider setting $PYTHONHOME to <prefix>[:<exec_prefix>]
'import site' failed; use -v for traceback
```

5) mod10.4 5_model_single.py

```
from modeller import *
from modeller.automodel import *
#from modeller import soap_protein_od

env = Environ()
a = AutoModel(env, alnfile='main_protein-7kiy.ali',
              knowns='7kiyA', sequence='main_protein',
              assess_methods=(assess.DOPE,
                              #soap_protein_od.Scorer(),
                              assess.GA341))
a.starting_model = 1
a.ending_model = 5
a.make()
```

```
$ mod10.4 5_model_single.py
Could not find platform independent libraries <prefix>
Could not find platform dependent libraries <exec_prefix>
Consider setting $PYTHONHOME to <prefix>[:<exec_prefix>]
'import site' failed; use -v for traceback
```

Check >> 5_model_single.log

```
>> Summary of successfully produced models:
Filename                          molpdf     DOPE score    GA341 score
------------------------------------------------------------------------
main_protein.B99990001.pdb    14399.21387  -161037.59375        1.00000
main_protein.B99990002.pdb    13218.66992  -163234.59375        1.00000
main_protein.B99990003.pdb    14407.94727  -160762.10938        1.00000
main_protein.B99990004.pdb    15190.11719  -160926.57812        1.00000
main_protein.B99990005.pdb    14338.67578  -161750.53125        1.00000
```

Note: Least DOPE score indicates the best model

6) mod10.4 6_evaluate_model.py

evaluate_model - Notepad

File Edit Format View Help

```
from modeller import *
from modeller.scripts import complete_pdb

log.verbose()    # request verbose output
env = Environ()
env.libs.topology.read(file='$(LIB)/top_heav.lib') # read topology
env.libs.parameters.read(file='$(LIB)/par.lib') # read parameters

# read model file
mdl = complete_pdb(env, 'main_protein.B99990002.pdb')

# Assess with DOPE:
s = Selection(mdl)   # all atom selection
s.assess_dope(output='ENERGY_PROFILE NO_REPORT', file='TvLDH.profile',
              normalize_profile=True, smoothing_window=15)
```

```
$ mod10.4 6_evaluate_model.py
Could not find platform independent libraries <prefix>
Could not find platform dependent libraries <exec_prefix>
Consider setting $PYTHONHOME to <prefix>[:<exec_prefix>]
'import site' failed; use -v for traceback
```