

MobyNet

<http://mobylenet.rpbs.univ-paris-diderot.fr>

Julien Maupetit, Pierre Tufféry.

-RPBS-

2009/11/13



- 1 The Mobylye Network
- 2 Tutorial - Homology modeling pipeline

The Mobyle Network

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- Structure
- Tests
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- lipm
- pasteur
 - alignment
 - structure
 - indexing
 - cosa

Data Bookmarks

Protein 3DAlignment: [refresh](#)

Ali2Modeller.pir

Protein 3DAlignment: [refresh](#)

Ali2Modeller.pir

Protein 3DAlignment: ali.data

Protein 3DAlignment: ali.data

Alignment: infile.data

BlastXMLReport: PDBBlast2-pdb.xml

PDB: 2weid.pdb

PDB: 3ek8A.pdb

PDB: 3ek8A.pdb

PDB: 3evrA.pdb

PDB: 3evuA.pdb

Protein PDB: result.pdb

Protein,DNA,RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

[refresh](#)

- HeligeneGetSequence - 11/28/09 15:17:50
- PDBBlast2 - 11/28/09 15:20:18
- XMLBlastSeq - 11/28/09 15:41:41

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HeligeneGetSequence@lipm PDBBlast2 XMLBlastSeq Clustalw: Multiple alignment@pasteur Ali2Modeller

Modeller Model applet use example plotSC **cosa@pasteur**

cosa@pasteur

Reset

Clustal ouput structural analysis ?

Run

* Alignment (Protein Alignment)

Paste File Result [clear data](#)

* Position in the sequence multialignment of the structure used as reference

* PDB entry (Protein Pdb)

Paste File [clear data](#)

Name of the output PDB file

Name of the output result file

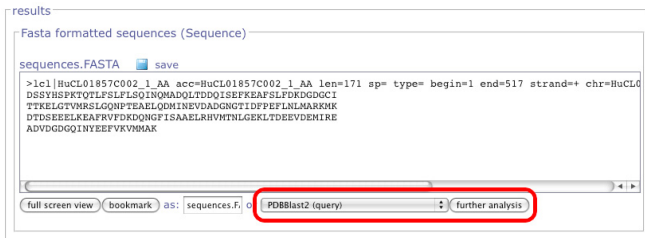
* : mandatory parameter

Author(s): T. Rose

Synopsis


We illustrate here how to take advantage of the Mobylenet to model the 3D structure of the sunflower protein corresponding to the HuCL01857C002 genomic information.

- tools at the three nodes (LIPM, Pasteur and RPBS) can be chained to complete the modeling
- *nota bene* : all calls are performed within the RPBS (remote imported services) portal



results

Fasta formatted sequences (Sequence)

sequences.FASTA  save

```
>1c1|HuCL01857C002_1_AA acc=HuCL01857C002_1_AA len=171 sp= type= begin=1 end=517 strand=+ chr=HuCL01857C002_1_AA
DSSYHSPKTQTLFSLFLSQINQADQLTDDQISEPKEAFSLFDRDGGDCI
TKELGTVMRSLGQNPTEAELQDMINEVDADGNGTIDFPFELNLMARKMK
DTDSEELKEAFRVFDKQNGFISAAELRHVMTNLGEKLTDEEVDEMIRE
ADVDDGGQINYEFPVKVMMK
```

full screen view bookmark as: sequences.F, 0 **PDBBlast2 (query)** further analysis

The full tutorial is available at :

<http://mobylenet.rpbs.univ-paris-diderot.fr/doc/tutorials/network.html>

Remote search for sunflower protein sequence

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Credits

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HeliGeneGetSequence@lipm x

HeliGeneGetSequence@lipm

Reset

Retrieve fasta sequences from HeliGene portal

Run

[Help Pages](#)

A list of HeliGene accessions (Text)

Paste | File [clear data](#)

Which type of data (clusters or peptides) to retrieve

Predicted peptides
 Mike Barker clusters

* : mandatory parameter

Author(s): Sebastien.Carrere@toulouse.inra.fr

Program help pages:

- <http://www.heliGene.org/>

Remote search for sunflower protein sequence

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HeliageneGetSequence@lipm x

HeliageneGetSequence@lipm

Reset Help Pages

Retrieve fasta sequences from Heliagene portal

Run

A list of Heliagene accessions (Text)

Paste File [clear data](#)

HuCL01857C002

Which type of data (clusters or peptides) to retrieve

Predicted peptides
 Mike Barker clusters

* : mandatory parameter

Author(s): Sebastien.Carrere@toulouse.inra.fr

Program help pages:

- <http://www.heliagene.org/>

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To validate your submission, please type the above text in the field below.

board

Cancel Ok

Heliagene portal

Kun

A list of Heliagene accessions (Text)

Paste File

clear data

HuCL01857C002

Which type of data (clusters or peptides) to retrieve

- Predicted peptides
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* : mandatory parameter

Author(s): Sebastien.Carrere@toulouse.inra.fr

Program help pages:

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Data Bookmarks

Text: accession.data

Jobs

✓ **HeliageneGetSequence - 11/28/09 15:17:50**

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HeliageneGetSequence 11/28/09 15:17:50

✓ <http://ilpm-bioinfo.toulouse.inra.fr/Mobyle/MobylePortal/tmp/HeliageneGetSequence/Q00696241210938>

results

-Fasta formatted sequences (Sequence)-

sequences.FASTA

```
>1c1|HuCL01857C002_1_AA acc=HuCL01857C002_1_AA len=171 sp= type= begin=1 end=517 strand++ chr=HuCL01857C002 def=IPR011992:EI
DSSVHSFKYQTLFSLFLSQINQADQLZDDQIISFKKFAFSLFDKDGDCI
TTRLEGTWRSLSGQNFTEALQDIMEVDADGNGTIDFPEFLNLRNRK
DTQSEEEKFAFVFDQNGTISAHELHVVWTLGKELTDEEVDKRE
ADVDDGQIINYEKFKVWNAK
```

as: sequences.F | <<>

parameters

-Which type of data (clusters or peptides) to retrieve (Choice)
 Value: peptides

-A list of Heliagene accessions (Text)

file	format detection program	re-formatted file
accession_data		

Command line
 /mnt/data10/www-heliagene/bin/int/misc/heliagene_get.pl --sequence --accession=accession_data --outfile=sequences.FASTA
 --type=peptides

job archive
[download this job as an archive](#)

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Data Bookmarks

Text: accession.data

Jobs

✓ **HeliageneGetSequence -**
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HeliageneGetSequence x
 11/28/09 15:17:50

✓ <http://lipm-bioinfo.toulouse.inra.fr/Mobyle/MobylePortal/tmp/HeliageneGetSequence/Q00696241210938>

results

Fasta formatted sequences (Sequence)

sequences.FASTA

```
>|c1|HuCL01857C002_1_AA acc=HuCL01857C002_1_AA len=171 sp= type= begin=1 end=517 strand=+ chr=HuCL01857C002 def=FR011992:EI
DSSVHSPKTYLFLSPLSQINQADQLTDDG1SEFRKAPSLPFDGDDGCI
TTKRELTPVHRSLSQNPTEAELQDMLNEVDADGNGCI DFFPFLMLMKRNR
DTSSEELKEAFVYFDQDQMF1SAELRNVYVNGEELTDEVDGEMIE
ADVDDGGQINYEYFKVYHAK
```

BS: sequences.Fj OF <>

parameters

Which type of data (clusters or peptides)
 Value: peptides

A list of Heliagene accessions (Text)

file **format detection program**

Command line

```
/mnt/data10/www-heliagene/bin/int/misc
--type=peptides
```

Job archive
[download this job as an archive](#)

MINI-FOLD (iSeq)
 MIR (iSeq)
 MUMmer (Sequence 1)
 MUMmer (Sequence 2)
 PDblast2 (query)
 PEP-FOLD-dev (iSeq)
 PEP-FOLD (iSeq)
 PredAcc ()
 ProFitv2_6 (all)
 ProbCons (Alignment)
 QMean (iSeq)
 SCSubstitute (iSeq)
 SCWRL (iSeq)
 SSpro (query)
 antiGENIC (sequence)
 backtransbig (sequence)
 backtransseq (sequence)
 banana (sequence)
 basibuilder-dev (query)
 basibuilder (query)

Search for a 3D template

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Data Bookmarks

Sequence: [sequences.FASTA](#) refresh

Text: [accession.data](#)

Jobs

HeliageneGetSequence - refresh
 11/28/09 15:17:50

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HeliageneGetSequence@lipm × PDBblast2 ×

PDBblast2

Two pass blast to search the PDB for homologues.

* Query (Protein Sequence)

Results bookmarks:

Paste

```

>|c1|HuCL01857C002_1_AA acc=HuCL01857C002_1_AA len=171 sp= type= begin=1 end=517 strand= chr=HuCL01857C002
def=IPR011992:EF-Hand type
DSYHSFPTQTLFSLFLSQIQMADQLTDDQISEPFAEFLFDKDGDCI
TTREELGTWRELQGNPTAEELQWMEINFDKNGDITDFEELNLSARIME
DTSDEELKEAFRVFDKQNGFISAAELRHVNTLGEKLTDEVENHIRE
ADVDDGQINIEEFVKVHMAK
          
```

First pass bank :

uniref100
 uniref90
 uniref50

Second pass bank :

pdbaa
 Astral-1.73-100
 Astral-1.73-95
 Astral-1.73-50

XML Output

* : mandatory parameter

Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaeffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), Gapped BLAST and PSI-BLAST: a new generation of protein database search programs, *Nucleic Acids Res.* 25:3389-3402.

Author(s): Altschul, Madden, Schaeffer, Zhang, Miller, Lipman. Two pass PSI-BLAST implemented by P. Tuffery

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Data Bookmarks

Sequence: sequences.FASTA refresh

Text: accession.date

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<http://mobyLe.rpbs.univ-paris-diderot.fr/data/jobs/PDBBlast2/Y00405683686018>

update job status | ask for help | back to program form | remove this job

parameters

Query (Protein Sequence)

file	format detection program	re-formatted file
sequences.FASTA (FASTA format)	squizz	

XML Output (Boolean)

Value: True

Command line

PDBBlast2 sequences.FASTA uniref90 pdbaa XML

Search for a 3D template

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Sequence: sequences.FASTA refresh
 Text: accession.data

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HeligeneGetSequence - refresh
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<http://mobyLe.rpbs.univ-paris-diderot.fr/data/jobs/PDBBlast2/Y00405683686018>

| | |

results

PDB blast report (BlastXMLReport)

PDBBlast2-pdb.xml

The file is too big to be safely displayed here.

| as: PDBBlast2-p or

Uniref blast report (BlastXMLReport)

PDBBlast2-uniref.xml

The file is too big to be safely displayed here.

| as: PDBBlast2-ur or

errors and warnings from PDBBlast2 (Text)

PDBBlast2_err

```
[blastppp] WARNING: a standard checkpoint file should have extension ".chk".
[blastppp] WARNING: -t larger than 1 not supported when restarting from a checkpoint; setting -t to 1
[blastppp] WARNING: [000.000] posReadCheckpoint: Attempting to recover data from previous checkpoint
[blastppp] WARNING: [000.000] posReadCheckpoint: Data recovered successfully
```

| as: PDBBlast2-er or

Select templates of interest

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BlastXMLReport: PDBBlast2 refresh

pdb.xml

Sequence: sequences.FASTA

Text: accession.data

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HeliageneGetSequence - refresh

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HeliageneGetSequence@lipm PDBBlast2 XMLBlastSeq x

XMLBlastSeq

Fetch blast hits sequences.

Reset

Run

Input Data

* Blast results (BlastXMLReport)

Paste File Result

edit data clear data

Results bookmarks: select

```
<?xml version="1.0"?>
<IDOCSTYPE BlastOutput PUBLIC "-//NCBI//NCBI BlastOutput/EN" "http://www.ncbi.nlm.nih.gov/dtd/NCBI_BlastOutput.dtd">
<BlastOutput>
  <blastOutput_program>blastp</blastOutput_program>
  <blastOutput_version>blastp 2.2.20 [Feb-08-2009]</blastOutput_version>
  <blastOutput_reference><Reference> Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), "Gapped BLAST and PSI-BLAST: a new generation of protein database
```

Your data cannot be fully displayed here since its size is too important

Filters

- * E-value threshold: 1e-70

* : mandatory parameter

Author(s): J. Maupetit

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▶ Multiple_Sequence_Com

▶ Retrieval

- ▶ HeligeneGetSequence
- ▶ SequenceAnalysis
- ▶ pasteur

Data Bookmarks

BlastXMLReport: PDBblast2-pdb.xml refresh

Sequence: sequences.FASTA

Text: accession.data

Jobs

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- ✓ **XMLBlastSeq - 11/28/09 15:41:41**

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HeligeneGetSequence 11/28/09 15:17:50 PDBblast2 11/28/09 15:20:18 XMLBlastSeq 11/28/09 15:41:41

✓ <http://mobyLe.rpbs.univ-paris-diderot.fr/data/jobs/XMLBlastSeq/W00585295721054>

[update job status](#) [ask for help](#) [back to program form](#) [remove this job](#)

results

XMLBlastSeq Results

Selected sequences (Protein or DNA or RNA Sequence)

XMLBlastSeq.fasta

```
>gi|218481831|pdb|3EK9|A Chain A, Calcium-Saturated Gomp2 T116vG87R MUTANT MONOMER
MRGRSHHHHMGASNTGQOQGRDLVDDDEKDLATVDSRRKRRKRGHAVRAIGRLESL
EMVYIMADKQKNGIKANFKIRHNIEDRGVQLAYHYQOQPTFGDGPVLLPDNHYLSVQKGL
SKDPHEKRDHYLLEFVTAAGITLGHDELKYGQGSNVSQGEELFGVVFILVELGDV
NGRHFVSGEGSDATVGRLELFICTGKELFVFWTLPTLWQCFNRYDMSQHF
KSAWPEGYIQERTIFFKDDCNKTRAEVYFEGDVLNRIELKGIQFKEDGNILGRKLEYN
TRDQLTEQIAEFKFAFSLFKDDGDTITKELQTVNRSIQNPTEAELQDINIYVDADG
NOTIDPFELTQIARRKSDTDSSEERFAEFVFDKDDGNYISAELRHVHTNLGKLTDE
EVDENIHEADIDGQVWTEFPQMTAK
```

full screen view | bookmark | as: XMLBlastSeq or <-> further analysis

standard output (Text)

XMLBlastSeq.out

```
# --
# XMLBlastSeq v0.2
# --
# Options:
# { 'debug': False, 'outFile': 'XMLBlast
# Arguments:
# { 'PDBblast2-pdb.xml' }
#
```

full screen view | bookmark | as: XMLBlastSeq or <-> further analysis

SeqLogo@lipm (sequences)
 IANTMultalinNucleic@lipm (sequence)
 IANTMultalinProtic@lipm (sequence)
 IANTPatScan@lipm (sequence)
 tululu@genouest (query_seq)
 EMBL@uniparis@pasteur (infile)

verbosity: False

Query/template sequence alignment

MobyLe@RPBS

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BlastXMLReport: PDBblast2-pdb.xml refresh

Protein,DNA,RNA Sequence:

XMLBlastSeq.fasta

Sequence: sequences.FASTA

Text: accession.data

Jobs

- ✓ HeligeneGetSequence - 11/28/09 15:17:50 refresh
- ✓ PDBblast2 - 11/28/09 15:20:18
- ✓ XMLBlastSeq - 11/28/09 15:41:41

Tutorials

- [How to use MobyLe? A step by step tutorial](#)
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- [Sequence formats](#)
- [Alignment formats](#)

Welcome | **Programs** | Data Bookmarks | Jobs | Tutorials

HeligeneGetSequence@lipm × PDBblast2 × XMLBlastSeq × Clustalw: Multiple alignment@pasteur ×

Clustalw: Multiple alignment@pasteur

Do full multiple alignment

Reset

Run

* Sequences File (a file containing several sequences) (-infile) (Sequence)

Paste

```

>|c1|HuCL01857C002_1_AA ace=HuCL01857C002_1_AA len=171 sp= type= chr= pm= def=IPR011992:EF-Hand type
DSYHEFTYGLTSLFLPSQIQWADQGLTQQIISSEFEATLELDKDGSGCI
TTLELCTVHRSLGQNPTEAELQOMINEVDAGNGTIDFPEFLNLMARKMK
DTDSEELKEAFRVFDKQNGFISAAELRHVMTNLGKLTDEEVDEMIIE
ADVDDGGQINTEEPFRVWMAK
>g1|z1P481811|pdb|3E8J|A Chain A, Calcium-Saturated Gomp2 T116vG87R MUTANT MONOMER
MRGSHHHHHHGMSNYGGQNGRDLYDDDDDLATVDSRRKWNKTGHAVRAIGRLSSL
ENYVIMADQKQNGIKANFKIRHIEDRGVQLAYHYQQNTPIDGQPVLLPNHYLSVQSKL
  
```

General settings

* Toggle Slow/Fast pairwise alignments (-quicktree) ?

Slow
 Fast

Protein or DNA (-type)

Multiple Alignments parameters ?

Gap opening penalty (-gapopen)

Gap extension penalty (-gapext)

No end gap separation penalty (-endgaps) ?

Gap separation penalty range (-gapdist) ?

Delay divergent sequences : % ident. for delay (-maxdiv) ?

File for new guide tree (-newtree)

Query/template sequence alignment

Mobyle@RPBS

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- ▼ lipm
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 - ▶ Multiple_Sequence_Com
 - ▼ Retrieval
 - ▶ HeliageneGetSequence
 - ▶ SequenceAnalysis
 - ▶ pasteur

Data Bookmarks

BlastXMLReport: PDBBlast2-pdb.xml refresh

Protein,DNA,RNA Sequence:
XMLblastSeq.fasta
Sequence: infile.data
Sequence: sequences.FASTA
Text: accession.data

Jobs

- ✓ HeliageneGetSequence - 11/28/09 15:17:50 refresh
- ✓ PDBBlast2 - 11/28/09 15:20:18
- ✓ XMLBlastSeq - 11/28/09 15:41:41
- ✓ clustalw-multialign - 11/28/09 15:44:11
- ✓ clustalw-multialign - 11/28/09 15:47:28

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- [How to use Mobyle? A step by step tutorial](#)
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✓ <http://mobyle.pasteur.fr/data/jobs/clustalw-multialign/R09457447350025>

results

Output parameters

Alignment file (Alignment)

infile_data.aln

```

lc1|uuCL01857C002_1_AA
*****
g1|217035445|pdb|3EYU|A|ISAAELRHVNTNLGKELTDEEVVDENIREADIDGGQVNYEEFVQMTAK
g1|217035444|pdb|3EYR|A|ISAAELRHVNTNLGKELTDEEVVDENIREADIDGGQVNYEEFVQMTA-
g1|218681835|pdb|3EKH|A|ISAAELRHVNTNLGKELTDEEVVDENIREADIDGGQVNYEEFVQMTAK
g1|218681831|pdb|3EK8|A|ISAAELRHVNTNLGKELTDEEVVDENIREADIDGGQVNYEEFVQMTAK
g1|226887604|pdb|2WEL|D|ISAAELRHVNTNLGKELTDEEVVDENIREADIDGGQVNYEEFVQMTAK
lc1|uuCL01857C002_1_AA
*****
  
```

as: or

Tree file (Tree)

infile_data.dnd

```

(
(
(
lc1|uuCL01857C002_1_AA:0.15716,
g1|226887604|pdb|2WEL|D:-0.05050)
:0.07049,
g1|218681831|pdb|3EK8|A:0.00021)
:0.00230,
g1|218681835|pdb|3EKH|A:0.00306)
  
```

as: or

standard output (Text)

clustalw-multialign.out

Query/template sequence alignment

Mobyle@RPBS

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Data Bookmarks

BlastXMLreport: PDBblast2-pdb.xml [refresh](#)

Protein, DNA, RNA Sequence:
 XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

HeligeneGetSequence - [refresh](#)
 11/28/09 15:17:50

✓ PDBblast2 - 11/28/09 15:20:18

✓ XMLBlastSeq - 11/28/09 15:41:41

✓ clustalw-multialign - 11/28/09 15:44:11

✓ clustalw-multialign - 11/28/09 15:47:28

Tutorials

- [How to use Mobyle? A step by step tutorial](#)
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HeligeneGetSequence 11/28/09 15:17:50 × PDBblast2 11/28/09 15:20:18 × XMLBlastSeq 11/28/09 15:41:41 × clustalw-multialign 11/28/09 15:44:11 × clustalw-multialign 11/28/09 15:47:28 ×

✓ <http://mobyle.pasteur.fr/data/jobs/clustalw-multialign/R09457447350025>

[update job status](#) | [ask for help](#) | [back to program form](#) | [remove this job](#)

results

Output parameters

Alignment file (Alignment) ?

infile_data.aln [save](#)

```

iE1|HuCl01857C002_1_AA
*****
g1|217035445|pdb|3EVU|A|ISAANELRHVHTNLGKELTDEEVDEHIREADIDGGQVNYEEFVQMTAK
g1|217035444|pdb|3EVN|A|ISAANELRHVHTNLGKELTDEEVDEHIREADIDGGQVNYEEFVQMTA-
g1|218681835|pdb|3EKN|A|ISAANELRHVHTNLGKELTDEEVDEHIREADIDGGQVNYEEFVQMTAK
g1|218681831|pdb|3EKN|A|ISAANELRHVHTNLGKELTDEEVDEHIREADIDGGQVNYEEFVQMTAK
g1|226887604|pdb|2WEL|D|ISAANELRHVHTNLGKELTDEEVDEHIREADIDGGQVNYEEFVQMTAK
iE1|HuCl01857C002_1_AA
*****
  
```

[full screen view](#) | [bookmark](#) as: infile_data.aln | [or](#) [further analysis](#)

Tree file (Tree)

infile_data.dnd [save](#)

```

(
(
(
iE1|HuCl01857C002_1_AA|0.15716,
g1|226887604|pdb|2WEL|D|-0.05050)
i0.07049,
g1|218681831|pdb|3EKN|A|i0.00021)
i0.00230,
g1|218681835|pdb|3EKN|A|i0.00306)
)
)
)
  
```

[full screen view](#) | [bookmark](#) as: infile_data.dnd | [or](#) [further analysis](#)

standard output (Text)

clustalw-multialign.out [save](#)

Preparing modeller input

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- ▶ pasteur

Data Bookmarks

Alignment: [infile_data.aln](#) refresh

BlastXMLReport: [PDBBlast2-pdb.xml](#)

Protein, DNA, RNA Sequence: [XMLBlastSeq.fasta](#)

Sequence: [infile.data](#)

Sequence: [sequences.FASTA](#)

Text: [accession.data](#)

Jobs

- ✓ HeliageneGetSequence - 11/28/09 15:17:50 refresh
- ✓ PDBBlast2 - 11/28/09 15:20:18
- ✓ XMLBlastSeq - 11/28/09 15:41:41
- ✓ clustalw-multialign - 11/28/09 15:44:11
- ✓ clustalw-multialign - 11/28/09 15:47:28

Tutorials

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- [Sequence formats](#)
- [Alignment formats](#)

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[HeliageneGetSequence@lipm](#) |
 [PDBBlast2](#) |
 [XMLBlastSeq](#) |
 [Clustalw: Multiple alignment@pasteur](#) |
 [Ali2Modeller](#) x

Ali2Modeller

Convert input alignment to Modeller PIR3D format.

Input Data

Input alignment (Alignment)

Paste | File | Result

|

Results bookmarks:

```

CLUSTAL 2.0.11 multiple sequence alignment
g1 217035445   pdb | 3EVU | A   HNGSHHHHHHGHASHTGGQGGRDLYDDDDKDLATHYDSSRRKWNKRGHA
g1 217035444   pdb | 3EVB | A   -----DSRRKWNKRGHA
g1 218681835   pdb | 3EK8 | A   HNGSHHHHHHGHASHTGGQGGRDLYDDDDKDLATHYDSSRRKWNKRGHA
g1 218681831   pdb | 3EK9 | A   HNGSHHHHHHGHASHTGGQGGRDLYDDDDKDLATHYDSSRRKWNKRGHA
          
```

Options

Fetch alignment PDB entries:

* : mandatory parameter

Author(s): J. Maupetit

Preparing modeller input

Mobile@RPBS

julien.maupetit@univ-paris-diderot.fr (guest)
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- ▼ ligm
- ▶ Analysis
- ▶ Annotations
- ▶ Multiple_Sequence_Com
- ▼ Retrieval
 - ▶ HeliageneGetSequence
 - ▶ SequenceAnalysis
 - ▶ pasteur

Data Bookmarks

Alignment: infile_data.aln refresh

BlastXMLReport: PDBBlast2-pdb.xml

Protein, DNA, RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile_data

Sequence: sequences.FASTA

Text: accession.data

Jobs

- ✓ **HeliageneGetSequence - 11/28/09 15:17:50** refresh
- ✓ **PDBBlast2 - 11/28/09 15:20:18**
- ✓ **XMLBlastSeq - 11/28/09 15:41:41**
- ✓ **clustalw-multialign - 11/28/09 15:44:11**
- ✓ **clustalw-multialign - 11/28/09 15:47:28**
- ✓ **Ali2Modeller - 11/28/09 15:49:00**

Welcome | **Programs** | **Data Bookmarks** | **Jobs** | **Tutorials**

HeliageneGetSequence 11/28/09 15:17:50 | PDBBlast2 11/28/09 15:20:18 | XMLBlastSeq 11/28/09 15:41:41 | clustalw-multialign 11/28/09 15:44:11 | clustalw-multialign 11/28/09 15:47:28

Ali2Modeller 11/28/09 15:49:00

✓ <http://mobile.rpbs.univ-paris-diderot.fr/data/jobs/Ali2Modeller/O00769200367928>

results

Ali2Modeller Results

Modeller PIR3D alignment (Protein 3DAlignment)

Ali2Modeller.pir

```
>P1;JevuA
structureX:JevuA:39:A:449:A::1:75:0:161
-----SSRRKKNKTHAVRAIGRLSEL
ENVYIMADQKMGKIKANFKIRHNIEDGGVQLAYHYQNTPIGGDFVLLFONHLYSTQGL
SKDPNEKRBHVLEFVTAAGITLGN-----SKGELPQGVFIVLVDGDV
HGHRFVSGDEGGDAFGKLLFLYICCTKGLPVPVPLVTLTI-VQCFRFBPHHQHDFP
KSAHPGQYIQENTFFKDDGNKTRAEVRFEGDGLVNRILKGIQFKEDGILGHKLSVM
T---LTSQYIAEFKFAFLFKDQDGTITTEKLEQVNRSLQNPTEALQMIENVADLG
NGTIDFPELTPMAKFKHDTDSEETIREFAFVFDKDGNGYISAALRHVHTNLGKLTDE
EVDENIREADIDGGQVNYEEFVQNTA--*
```

as: Ali2Modeller or

Template PDB file (Protein PDB)

JevuA.pdb

```
HEADER
ATOM 1 N SER A 39 -24.963 0.378 58.321 1.00 47.27 N
ATOM 2 CA SER A 39 -24.917 -1.010 57.885 1.00 41.96 C
ATOM 3 C SER A 39 -25.944 -1.317 56.798 1.00 31.79 C
ATOM 4 O SER A 39 -25.964 -2.422 56.264 1.00 26.56 O
ATOM 5 CB SER A 39 -25.129 -1.958 59.063 1.00 41.99 C
ATOM 6 OG SER A 39 -24.919 -3.300 58.665 1.00 43.73 O
ATOM 7 N SER A 40 -26.813 -0.358 56.494 1.00 27.16 N
ATOM 8 CA SER A 40 -27.684 -0.488 55.330 1.00 23.86 C
ATOM 9 C SER A 40 -26.835 -0.553 54.072 1.00 26.79 C
```

as: JevuA.pdb or

3ekhA.ntdb

Preparing modeller input

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 - ▶ HeligeneGetSequence
 - ▶ SequenceAnalysis
 - ▶ pasteur

Data Bookmarks

Alignment: infile_data.aln refresh

BlastXMLReport: PDBblast2-pdb.xml

Protein,DNA,RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

- ▶ HeligeneGetSequence - 11/28/09 15:17:50 refresh
- ▶ PDBblast2 - 11/28/09 15:20:18
- ▶ XMLBlastSeq - 11/28/09 15:41:41
- ▶ clustalw-multialign - 11/28/09 15:44:11
- ▶ clustalw-multialign - 11/28/09 15:47:28
- ▶ Ali2Modeller - 11/28/09 15:49:00

Tutorials

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 PDBblast2 11/28/09 15:20:18 |
 XMLBlastSeq 11/28/09 15:41:41 |
 clustalw-multialign 11/28/09 15:44:11 |
 clustalw-multialign 11/28/09 15:47:28

Ali2Modeller 11/28/09 15:49:00 x

<http://mobyLe.rpbs.univ-paris-diderot.fr/data/Jobs/Ali2Modeller/O00769200367928>
update job status | ask for help | back to program form | remove this job

results

Ali2Modeller Results

Modeller PIR3D alignment (Protein 3DAlignment)

Ali2Modeller.pir save

```
>P1;3evuA
structureX:3evuA:39:A:449:A::1.75:0.161
-----ESRRKMKNGHAYRAIGRLSGL
EMVFLHADKQKNGIRANFKIRBIEGGVQLATHYQQGPTIGDGFVLLPDSHYLSTQKFL
SRDFMERGGHYLLEFYTAGITLGG-----SRGELFPGVYFTLVELDQVY
NGHKFVSVSGEGDATTGKLTGKLFICTTGKLPVFWTLVITL-VQCFSRYPDHNKQDFF
KSAFPGYIQERTIPFKDDQNYKTRAEVRFEGDGLVNRLELNGLDPRDQNLGKLEYN
T---LTERQLAEFKFKAFLPFDKDDGDTITTKRELQVYRSLQGHITAEELQGHINEVDAG
NGTIDDFPEFLTHMKRKHDFDSEERIEAFKRVFDKDGNGYISAAELRHVMTNLEKLTDE
EVDEHIREADIDGGQVYVEEFVQMPTA--*
```

full screen view | bookmark | as: Ali2Modeller | or <> | further analysis
< | > | Modeller (all)

Template PDB file (Protein PDB)

3evuA.pdb save

```
HEADER
ATOM      1  N  SER  A  39      -24.963   0.378  58.321   1.00  47.27   N
ATOM      2  CA  SER  A  39      -24.917  -1.010  57.885   1.00  41.96   C
ATOM      3  C  SER  A  39      -25.944  -1.317  56.798   1.00  31.79   C
ATOM      4  O  SER  A  39      -25.964  -2.422  56.264   1.00  26.56   O
ATOM      5  CB  SER  A  39      -25.129  -1.958  59.063   1.00  41.99   C
ATOM      6  OG  SER  A  39      -24.919  -3.300  58.665   1.00  43.73   O
ATOM      7  N  SER  A  40      -26.813  -0.358  56.494   1.00  27.16   N
ATOM      8  CA  SER  A  40      -27.684  -0.488  55.330   1.00  23.86   C
ATOM      9  C  SER  A  40      -26.835  -0.553  54.072   1.00  26.79   C
```

full screen view | bookmark | as: 3evuA.pdb | or <> | further analysis

3ekh.pdb save

```
HEADER
3EKH
```


Perform the 3D modeling

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- Retrieval
- HeliageneGetSequence
- SequenceAnalysis
- pasteur

Data Bookmarks

Protein 3DAlignment: refresh

All2Modeller.pir

Alignment: infile_data.aln

BlastXMLReport: PDBblast2-pdb.xml

PDB: 2weId.pdb

PDB: 3ekhA.pdb

PDB: 3ekhA.pdb

PDB: 3evrA.pdb

PDB: 3evrA.pdb

Protein_DNA_RNA_Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

HeliageneGetSequence - refresh

11/28/09 15:17:50

PDBblast2 - 11/28/09 15:20:18

XMLBlastSeq - 11/28/09 15:41:41

clustalw-multialion -

Welcome Programs Data Bookmarks Jobs Tutorials

HeliageneGetSequence@lipm PDBblast2 XMLBlastSeq Clustalw: Multiple alignment@pasteur All2Modeller

Modeller x

Modeller

Reset

Help Pages

Run

Input Data

* MODELLER Licence Key ? [xxxxxx]

* Input alignment (Protein 3DAlignment) ?

Paste File Result

edit data clear data

Results bookmarks: <-> select

```
>P1;3evuA
structureX:3evuA:39:A:449:A::1:75:0:161
-----SRRRKWKTKHAVAIGRLSEI
ENVYIMADKQKNGIKANFKIRHNIEDGQVQLAYHYQNTPIGDGPULLPDHNYLSTQSKL
SKDPNEKRDHNVLLEFVTAAGITLGH-----SKGEELPTGVVPILVELDGDV
NQRKFSVSGEGDATYKGLTLKFICTGKLPVWPFLVITL-VQCFRYPDMRRQSDHF
KRAMPEQYIQERTIFFKDDGNTKRAEVKFFEDQLVWRLELGGIDPFKEDNLIQKLEVN
```

* Template structure (Protein PDB) ?

Paste DB File

edit data clear data

File Bookmarks: <-> select

HEADER								2WEI			
ATOM	2449	N	ASP	D	3	77.230	-15.382	-66.932	1.00	37.71	N
ATOM	2450	CA	ASP	D	3	76.423	-15.307	-68.311	1.00	45.81	C
ATOM	2451	C	ASP	D	3	77.456	-16.094	-69.335	1.00	47.60	C
ATOM	2452	O	ASP	D	3	76.928	-16.927	-70.082	1.00	47.58	O
ATOM	2453	CB	ASP	D	3	76.477	-13.843	-68.764	1.00	43.86	C
ATOM	2454	CG	ASP	D	3	75.016	-13.413	-68.965	1.00	54.82	C

Models to build ? [5-15]

Perform the 3D modeling

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 - ▶ SequenceAnalysis
- ▶ pasteur

Data Bookmarks refresh

Protein 3DAlignment: [refresh](#)

Ali2Modeller.pir

Protein 3DAlignment:

Ali2Modeller.pir

Protein 3DAlignment: ali.data

Protein 3DAlignment: ali.data

Alignment: infile_data.aln

BlastXMLReport: PDBBlast2-pdb.xml

PDB: 2weid.pdb

PDB: 3ek8a.pdb

PDB: 3ek8a.pdb

PDB: 3evrA.pdb

PDB: 3evuA.pdb

Protein_DNA_RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

Welcome | **Programs** | **Data Bookmarks** | **Jobs** | **Tutorials**

HeliageneGetSequence 11/28/09 15:17:50	PDBBlast2 11/28/09 15:20:18	XMLBlastSeq 11/28/09 15:41:41	clustalw-multialign 11/28/09 15:44:11	clustalw-multialign 11/28/09 15:47:28
Ali2Modeller 11/28/09 15:49:00	Modeller 11/28/09 15:54:30	Modeller 11/28/09 15:56:21	Modeller 11/28/09 15:57:20	Ali2Modeller 11/28/09 16:04:05

Modeller
11/28/09 16:05:45

✓ <http://mobyLe.rpbs.univ-paris-diderot.fr/data/jobs/Modeller/H00977427918911>

[update job status](#) | [ask for help](#) | [back to program form](#) | [remove this job](#)

results

Modeller Results

Modeller ouput (Protein PDB)

Modeller-MobyLe-01.pdb [save](#)

```

EXPDTA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07:10
REMARK 6 MODELLER OBJECTIVE FUNCTION: 20031.1191
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000
ATOM 1 N SER 1 78.504 -33.259 -55.210 1.00 74.86 N
ATOM 2 CA SER 1 78.854 -34.923 -53.995 1.00 74.86 C
ATOM 3 CB SER 1 79.279 -35.451 -54.372 1.00 74.86 C
ATOM 4 OG SER 1 78.200 -36.144 -54.977 1.00 74.86 O
ATOM 5 C SER 1 80.005 -33.385 -53.304 1.00 74.86 C
ATOM 6 O SER 1 79.597 -32.192 -53.009 1.00 74.86 O
ATOM 7 N SER 2 81.037 -34.194 -53.018 1.00 35.44 N
  
```

[full screen view](#) | [bookmark](#) as: Modeller-Mo or <> [further analysis](#)

Modeller-MobyLe-04.pdb [save](#)

```

EXPDTA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:10:33
REMARK 6 MODELLER OBJECTIVE FUNCTION: 20383.7676
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000
ATOM 1 N SER 1 78.888 -34.393 -55.123 1.00 74.18 N
ATOM 2 CA SER 1 78.749 -33.689 -54.435 1.00 74.18 C
ATOM 3 CB SER 1 77.701 -33.179 -53.314 1.00 74.18 C
ATOM 4 OG SER 1 78.177 -34.004 -52.262 1.00 74.18 O
ATOM 5 C SER 1 80.047 -32.703 -53.820 1.00 74.18 C
ATOM 6 O SER 1 80.296 -31.531 -53.550 1.00 74.18 O
ATOM 7 N SER 2 80.521 -33.696 -53.583 1.00 79.86 N
  
```

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Perform the 3D modeling

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- ▼ Retrieval
 - ▶ HeligeneGetSequence
 - ▶ SequenceAnalysis
- ▶ pasteur

Data Bookmarks

Protein 3DAlignment: refresh

All2Modeller.pir

Protein 3DAlignment:

All2Modeller.pir

Protein 3DAlignment: all.data

Protein 3DAlignment: all.data

Alignment: infile_data.aln

BlastXMLReport: PDBblast2-pdb.xml

PDB: 2weld.pdb

PDB: 3ek8A.pdb

PDB: 3ekhA.pdb

PDB: 3evrA.pdb

PDB: 3evuA.pdb

Protein_DNA_RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile_data

Sequence: infile_data

Sequence: sequences.FASTA

Text: accession.data

Jobs

- ✓ HeligeneGetSequence - refresh
- 11/28/09 15:17:50
- ✓ PDBblast2 - 11/28/09 15:20:18

Welcome Programs Data Bookmarks **Jobs** Tutorials

HeligeneGetSequence 11/28/09 15:17:50	PDBblast2 11/28/09 15:20:18	XMLBlastSeq 11/28/09 15:41:41	clustalw-multialign 11/28/09 15:44:11	clustalw-multialign 11/28/09 15:47:28
All2Modeller 11/28/09 15:49:00	Modeller 11/28/09 15:54:30	Modeller 11/28/09 15:56:21	Modeller 11/28/09 15:57:20	All2Modeller 11/28/09 16:04:05
Modeller 11/28/09 16:05:45	Modeller 11/28/09 16:25:21	Modeller 11/28/09 16:27:14		

✓ <http://mobyle.rpbs.univ-paris-diderot.fr/data/jobs/Modeller/H00977427918911>

results

Modeller Results

Modeller output (Protein PDB)

Modeller-Mobyle-01.pdb

```

EXPDTA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07:10
REMARK 6 MODELLER OBJECTIVE FUNCTION: 20031.1191
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000
ATOM 1 N SER 1 78.504 -33.259 -55.210 1.00 74.86 N
ATOM 2 CA SER 1 78.854 -34.023 -53.995 1.00 74.86 C
ATOM 3 CB SER 1 79.279 -35.451 -54.372 1.00 74.86 C
ATOM 4 OG SER 1 78.200 -36.144 -54.977 1.00 74.86 O
ATOM 5 C SER 1 80.005 -33.385 -53.304 1.00 74.86 C
ATOM 6 O SER 1 79.997 -32.192 -53.009 1.00 74.86 O
ATOM 7 N SER 2 81.037 -34.194 -53.018 1.00 35.44 N
  
```

Modeller-Mobyle-04.pdb

```

EXPDTA THEORETICAL MODEL, MODELLER
REMARK 6 MODELLER OBJECTIVE FUNCTION:
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID:
ATOM 1 N SER 1 78.888 SCSubstitute (ipdb) 18 N
ATOM 2 CA SER 1 78.745 SCWRL (IPDB) 18 C
ATOM 3 CB SER 1 77.703 TIF (POB) 18 C
ATOM 4 OG SER 1 78.175 sup (query) 18 O
ATOM 5 C SER 1 80.044 extractTurn (query) 18 C
ATOM 6 O SER 1 80.294 fpocket (query) 18 O
ATOM 7 N SER 2 80.923 Superpose (moving) 86 N
Superpose (reference)
  
```

Modeller-Mobyle-05.pdb

```

EXPDTA THEORETICAL MODEL, MODELLER
REMARK 6 MODELLER OBJECTIVE FUNCTION:
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000
  
```

A quick glance at the 3D model

MobyLe@RPBS

julien.maupetit@univ-paris-diderot.fr (guest)
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 - ▶ Multiple_Sequence_Com
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 - ▶ HeliGeneGetSequence
 - ▶ SequenceAnalysis
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Data Bookmarks refresh

- Protein 3DAlignment: [refstht](#)
- All2Modeller.pir
- Protein 3DAlignment: [ali.data](#)
- All2Modeller.pir
- Protein 3DAlignment: [ali.data](#)
- Protein 3DAlignment: [ali.data](#)
- Alignment: [infile_data.aln](#)
- BlastXMLReport: [PDBBlast2-pdb.xml](#)
- PDB: [2welD.pdb](#)
- PDB: [3ek8A.pdb](#)
- PDB: [3ekhA.pdb](#)
- PDB: [3evrA.pdb](#)
- PDB: [3evuA.pdb](#)
- Protein PDB: [Modeller-MobyLe-01.pdb](#)
- Protein,DNA,RNA Sequence: [XMLBlastSeq.fasta](#)
- Sequence: [infile_data](#)
- Sequence: [infile_data](#)
- Sequence: [sequences.FASTA](#)
- Text: [accession.data](#)

Welcome **Programs** Data Bookmarks Jobs Tutorials

HeliGeneGetSequence@lipm × PDBBlast2 × XMLBlastSeq × Custalw: Multiple alignment@pasteur × All2Modeller ×

Modeller × Jmol applet use example ×

Jmol applet use example

Reset

Jmol applet 3D viewer.

Run

Paragraph Test

Parameter 1 (PDB)

Paste DB File Result

edit data clear data

Results bookmarks: select

```

EXPDTA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07:10
REMARK 6 MODELLER OBJECTIVE FUNCTION: 20031.1191
REMARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000
ATOM 1 N SER 1 78.504 -33.259 -55.210 1.00 74.86 N
ATOM 2 CA SER 1 78.854 -34.023 -53.995 1.00 74.86 C
ATOM 3 CB SER 1 79.279 -35.451 -54.372 1.00 74.86 C
ATOM 4 OG SER 1 78.200 -36.144 -54.977 1.00 74.86 O
  
```

* : mandatory parameter

Reference: *Jmol: an open-source Java viewer for chemical structures in 3D.* <http://www.jmol.org/>

Author(s):

A quick glance at the 3D model

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 - ▶ Analysis
 - ▶ Annotations
 - ▶ Multiple_Sequence_Com
 - ▼ Retrieval
 - ▶ HeliageneGetSequence
 - ▶ SequenceAnalysis
 - ▶ pasteur

Data Bookmarks

Protein 3DAlignment: [refresh](#)

Ali2Modeller.pir

Protein 3DAlignment:

Ali2Modeller.pir

Protein 3DAlignment: all.data

Protein 3DAlignment: all.data

Alignment: infile_data.aln

BlastXMLReport: PDBBlast2-pdb.xml

PDB: 2weId.pdb

PDB: 3ek8A.pdb

PDB: 3ekhA.pdb

PDB: 3evrA.pdb

PDB: 3evuA.pdb

Protein PDB: Modeller-Mobyle-01.pdb

Protein_DNA_RNA Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

HeliageneGetSequence - [refresh](#)

- ✓ 11/28/09 15:17:50
- ✓ PDBBlast2 - 11/28/09 15:20:18

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HeliageneGetSequence 11/28/09 15:17:50	PDBBlast2 11/28/09 15:20:18	XMLBlastSeq 11/28/09 15:41:41	clustalw: multialign 11/28/09 15:44:11	clustalw: multialign 11/28/09 15:47:28
Ali2Modeller 11/28/09 15:49:00	Modeller 11/28/09 15:54:30	Modeller 11/28/09 15:56:21	Modeller 11/28/09 15:57:20	Ali2Modeller 11/28/09 16:04:05
Modeller 11/28/09 16:05:45	Modeller 11/28/09 16:25:21	Modeller 11/28/09 16:27:14	jmol_example 11/28/09 16:28:44	

✓ http://mobyle.rpbs.univ-paris-diderot.fr/data/jobs/jmol_example/Z01816957216978

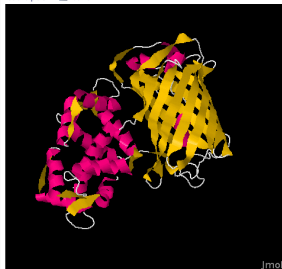
[update job status](#) [ask for help](#) [back to program form](#) [remove this job](#)

results

Results Paragraph

Jmol structure viewer (PDB)

result.pdb [save](#)



```
EXFPYA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07
REMARK 6 MODELLER OBJECTIVE FUNCTION: 28031.1191
REMARK 6 MODELLER BEST TEMPLATE & SEQ ID: 100.000
ATOM 1 N SER 1 78.504 -33.259 -55.210 1.
ATOM 2 CA SER 1 78.854 -34.023 -53.995 1.
ATOM 3 CB SER 1 79.279 -35.451 -54.372 1.
ATOM 4 OG SER 1 78.200 -36.144 -54.977 1.
ATOM 5 C SER 1 80.005 -33.385 -53.304 1.
ATOM 6 O SER 1 79.997 -32.192 -53.009 1.
```

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A quick glance at the 3D model

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 - SequenceAnalysis
 - pasteur

Data Bookmarks

Protein 3DAlignment: result.pdb refresh

Protein 3DAlignment: pir

Protein 3DAlignment: all2Modeller.pir

Protein 3DAlignment: all.data

Protein 3DAlignment: all.data

Alignment: infile_data.aln

BlastXMLReport: PDBBlast2-pdb.xml

PDB: 2weID.pdb

PDB: 3ek8A.pdb

PDB: 3ekhA.pdb

PDB: 3evrA.pdb

PDB: 3evuA.pdb

Protein PDB: result.pdb

Protein_DNA_RNA Sequence: XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Jobs

- HeliageneGetSequence - 11/28/09 15:17:50 refresh
- PDBBlast2 - 11/28/09 15:20:18
- XMLBlastSeq - 11/28/09 15:41:41
- clustalw-multialign 11/28/09 15:44:11
- clustalw-multialign 11/28/09 15:47:28
- All2Modeller 11/28/09 15:49:00
- Modeller 11/28/09 15:54:30
- Modeller 11/28/09 15:56:21
- Modeller 11/28/09 15:57:20
- All2Modeller 11/28/09 16:04:05
- Modeller 11/28/09 16:05:45
- Modeller 11/28/09 16:25:21
- Modeller 11/28/09 16:27:14
- jmol_example 11/28/09 16:28:44

Welcome	Programs	Data Bookmarks	Jobs	Tutorials
HeliageneGetSequence 11/28/09 15:17:50	PDBBlast2 11/28/09 15:20:18	XMLBlastSeq 11/28/09 15:41:41	clustalw-multialign 11/28/09 15:44:11	clustalw-multialign 11/28/09 15:47:28
All2Modeller 11/28/09 15:49:00	Modeller 11/28/09 15:54:30	Modeller 11/28/09 15:56:21	Modeller 11/28/09 15:57:20	All2Modeller 11/28/09 16:04:05
Modeller 11/28/09 16:05:45	Modeller 11/28/09 16:25:21	Modeller 11/28/09 16:27:14	jmol_example 11/28/09 16:28:44	

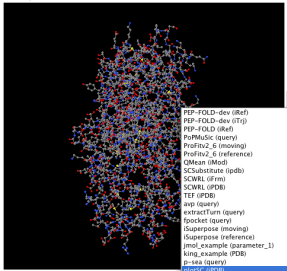
http://mobyle.rpbs.univ-paris-diderot.fr/data/jobs/jmol_example/Z01816957216978

results

Results Paragraph

Jmol structure viewer (PDB)

result.pdb



EXPDTA THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07

MARK 6 MODELLER OBJECTIVE FUNCTION: 20031.1191

MARK 6 MODELLER BEST TEMPLATE % SEQ ID: 100.000

DM	N	SER	1	78.504	-33.259	-55.210	1.	
DM	2	CA	SER	1	78.854	-34.023	-53.995	1.
DM	3	CB	SER	1	79.279	-35.451	-54.372	1.
DM	4	OG	SER	1	78.200	-36.144	-54.977	1.
DM	5	C	SER	1	80.005	-33.385	-53.304	1.
DM	6	O	SER	1	79.997	-32.192	-53.009	1.

as: result.pdb or plotSC (PDB)

Any further analysis ?

MobyLe@RPBS

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Data Bookmarks refresh

Protein 3DAlignment: [Ali2Modeller.pir](#)

Protein 3DAlignment: [Ali2Modeller.pir](#)

Protein 3DAlignment: [ali.data](#)

Protein 3DAlignment: [ali.data](#)

Alignment: [infile_data.aln](#)

BlastXMLReport: [PDBblast2-pdb.xml](#)

PDB: [2weID.pdb](#)

PDB: [3ek8A.pdb](#)

PDB: [3ekhA.pdb](#)

PDB: [3evrA.pdb](#)

PDB: [3evuA.pdb](#)

Protein PDB: [result.pdb](#)

Protein,DNA,RNA Sequence: [XMLBlastSeq.fasta](#)

Sequence: [infile.data](#)

Sequence: [infile.data](#)

Sequence: [sequences.FASTA](#)

Text: [accession.data](#)

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HeliageneGetSequence@lipm | PDBblast2 | XMLBlastSeq | Chustalw: Multiple alignment@pasteur | Ali2Modeller

Modeller | Jmol applet use example | **plotSC** | x

plotSC

Reset

Help Pages

Scit: Chis plots ?

Run

Input Data

* Input PDB file (PDB)

Paste

Results bookmarks:

EXPDTA	THEORETICAL MODEL, MODELLER 9v6 2009/11/28 16:07:10						
REMARK	6 MODELLER OBJECTIVE FUNCTION: 20031.1191						
REMARK	6 MODELLER BEST TEMPLATE % SEQ ID: 100.000						
ATOM	1	N	SER	1	78.504 -33.259 -55.210	1.00 74.86	N
ATOM	2	CA	SER	1	78.854 -34.023 -53.995	1.00 74.86	C
ATOM	3	CB	SER	1	79.279 -35.451 -54.372	1.00 74.86	C
ATOM	4	OG	SER	1	78.200 -36.144 -54.977	1.00 74.86	O

* : mandatory parameter

Reference: SCit: web tools for protein side chain conformation analysis. Gautier R, Camproux AC, Tuffery P. Nucleic Acids Res. 2004 Jul 1;32(Web Server issue):W508-11.

Author(s): Gautier R

Program help pages:

- <http://bioserv.rpbs.univ-paris-diderot.fr/Help/SCitHelp.html>

Any further analysis?

Moby@RPBS

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genouest

lipm

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Annotations

Multiple_Sequence_Com

Retrieval

- ▶ HeliageneGetSequence
- ▶ SequenceAnalysis

pasteur

Data Bookmarks

Protein 3DAlignment: refresh

All2Modeller.pir

Protein 3DAlignment:

All2Modeller.pir

Protein 3DAlignment: all.data

Protein 3DAlignment: all.data

Alignment: infile_data.aln

BlastXMLReport: PDBBlast2-pdb.xml

PDB: 2welD.pdb

PDB: 3ek8A.pdb

PDB: 3ekhA.pdb

PDB: 3evrA.pdb

PDB: 3evrA.pdb

Protein PDB: result.pdb

Protein_DNA_RNA_Sequence:

XMLBlastSeq.fasta

Sequence: infile.data

Sequence: infile.data

Sequence: sequences.FASTA

Text: accession.data

Welcome	Programs	Data Bookmarks	Jobs	Tutorials
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All2Modeller 11/28/09 15:49:00	Modeller 11/28/09 15:54:30	Modeller 11/28/09 15:56:21	Modeller 11/28/09 15:57:20	All2Modeller 11/28/09 16:04:05
Modeller 11/28/09 16:05:45	Modeller 11/28/09 16:25:21	Modeller 11/28/09 16:27:14	jmol_example 11/28/09 16:28:44	plotSC 11/28/09 16:31:23

✓ <http://mobyte.rpbs.univ-paris-diderot.fr/data/jobs/plotSC/K02302377928972>

[update job status](#) [ask for help](#) [back to program form](#) [remove this job](#)

results

Output

Plot files (Picture)

FigSCpr-VAL.jpeg [save](#)



[full screen view](#) [bookmark](#) as: FigSCpr-VAL

FigSCpr-ILE.jpeg [save](#)



[full screen view](#) [bookmark](#) as: FigSCpr-ILE

Summary

