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| MolTK | |
|  | moltk1 |
|  | User’s Manual |
|  | Release 0.3.4  December 20, 2007 |
|  | Website: rotatingpenguin.com/moltk |

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**Acknowledgments**

Special thanks to Joy Ku who created the beautiful template for this manual. Thanks also to Christopher D. Putnam and Robert Edgar for helpful discussions about sequence alignment.

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# Introduction to MolTK

## Overview

### What is MolTK?

There are three faces of MolTK; in order from easiest-to-use to most-powerful:

1. MolTK is a computer application that allows the user to view and align molecular sequences and structures.
2. Moltk is a Python programming language module that allows the user to align and otherwise compute on molecular sequences and structures.
3. Moltk is a C++ API that allow the programmer to compute with molecular sequences and structures with high efficiency.

### Design Goals of MolTK

* Python programming language interactive environment for sequence/structure alignment that is just as easy to use as our (aging) dedicated alignment tool SEQUOIA.
* Flexible architecture that makes it easy to experiment with custom alignment methods and scoring systems.
* Consistent, well documented API for both Python and C++ programmers.
* Units-aware quantity type system. Thus alignment scores are not just numbers, they are information quantities with units of "bits". Atomic coordinates are not just numbers x, y, z, but are vector quantities with units of nanometers. Units-aware quantity types are an important part of scientific computing hygiene:
  + Converting a "quantity" to a raw number requires a "unit" to express the quantity in. This requires the user to pay attention to units at precisely the moment when knowing the unit is most important. The rest of the time is "just works", even if you are wrong about what the current units are!
  + This sort of type safety in scientific computing might help prevent errors such as, say, crashing $100 million orbiters into planets.
  + Type safety: Adding a length to a volume makes no sense, and will result in an error. Dividing a length by a time results in a velocity.
* Next-generation molecular sequence/structure viewer that adheres to our user interface principles.

## Installing MolTK

MolTK download site: <http://code.google.com/p/moltk/downloads/list>

### Installing the MolTK Application

### Installing the MolTK Python Module

### Installing the MolTK C++ SDK

### Building MolTK from Source Code

## Software License

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Commercial users should ask about our dual licensing model.

For questions contact: cmbruns@rotatingpenguin.com

## Resources

Browse the MolTK home page at:

http://rotatingpenguin.com/moltk/

Download MolTK at:

http://code.google.com/p/moltk/downloads/list

Find questions and answers in the moltk-users forum at:

http://groups.google.com/group/moltk-users

Report issues and get the source code at:

http://code.google.com/p/moltk/

Study the MolTK Python API at:

http://www.rotatingpenguin.com/moltk/api\_python/python\_api.html

Study the MolTK C++ API at:

http://www.rotatingpenguin.com/moltk/api\_cxx/cxx\_api.html

# The MolTK Application

# Programming MolTK

## Python

### Tutorial

Download and install MolTK from the MolTK download site:

<http://code.google.com/p/moltk/downloads/list>

In the following examples text following the >>> prompt represents

commands typed by the user. Other lines represent the output of the program.

#### Scenario 1: Aligning 3 Sequences

In this example, the files test1.fasta, test2.fasta, and test3.fasta are sequences in the FASTA format. Information about the FASTA format can be found at

<http://www.ncbi.nlm.nih.gov/BLAST/blastcgihelp.shtml>. A file called test.fasta can be saved with the alignment. The alignment can be also saved as test.pretty which is a nicely formatted but not computer parseable version of the alignment. What follows is an example of performing an alignment of three sequences.

##### Step 1. Download FASTA Test Sequences

Go to download page <http://code.google.com/p/moltk/downloads/list> and download

the three test sequences: test1.fasta, test2.fasta, and test3.fasta.

##### Step 2. Start an Alignment Session

% python -i

>>> **import** moltk

##### Step 3. Load test1.fasta Sequence into Seq1

>>> seq1 = moltk.load\_fasta**(**"test1.fasta"**)**

##### Step 4. Load test2.fasta Sequence into Seq2

>>> seq2 = moltk.load\_fasta**(**"test2.fasta"**)**

##### Step 5. Align Seq1 and Seq2

>>> align1 = moltk.align**(**seq1, seq2**)**

##### Step 6. Display the Alignment on the Screen

>>> **print** align1

##### Step 7. Load test3.fasta Sequence into Seq3

>>> seq3 = moltk.load\_fasta**(**"test3.fasta"**)**

##### Step 8. Align Previous Alignment of test1.fasta and test2.fasta with test3.fasta

>>> align2 = moltk.align**(**align1, seq3**)**

##### Step 9. Save the Alignment to a File

>>> align2.write\_fasta**(**"test.fasta"**)**

You can also save as test.pretty for a nicely formatted but not computer parseable version.

>>> align2.write\_pretty**(**"test.pretty"**)**

##### Step 10. Display a Table of Pairwise Sequence Identities

>>> **print** align2.id\_table**()**

##### Step 11. End Your Alignment Session

>>> quit**()**

#### Scenario 2: Writing a Python Script to Help Automate the Alignment Process

#### Scenario 3: Aligning 2 Sequences and Assessing Significance

#### Scenario 4: Overlaying 2 tertiary structures

### MolTK for SEQUOIA Users

## C++

### MolTK Coding Style Guidelines

Purpose: To provide a consistent look for both python and C++ MolTK code.

#### Indentation

Use four space characters per indent. No tabs.

#### Class names

Use CapitalizedWords

Use all caps for abbreviations, e.g. PDBStructure.

Class names should be nouns.

#### Macro, enum, and constant names

CAPITALIZED\_WITH\_UNDERSCORES

#### Method and function names

Use lower\_case\_with\_underscores.

Begin method and function names with a verb.

#### Attribute and member names

lower\_case\_with\_underscores

adjective\_noun or noun

b\_variable\_name for boolean values

#### Namespace, package, and module names

lower case, single word, short names

#### Method parameters

lower\_case\_with\_underscores

Remember that method parameter names are more important in python than in C++, because python allows named parameter use. In all C++ header files, every parameter to every exposed method should have an understandable name.

# Bibliography

Dayhoff, M. O., 1969. *Atlas of Protein Sequence and Structure.* Silver Spring, MD: National Biomedical Research Foundation.

Edgar, R. C., 2004. MUSCLE: multiple sequence alignment with high accuracy and high throughput. *Nucleic Acids Research,* 32(5), pp. 1792-1797.

Gusfield, D., 1997. *Algorithms on Strings, Trees, and Sequences.* Cambridge: Cambridge University Press.

Henikoff, S. & Henikoff, J. G., 1992. Amino acid substitution matrices from protein blocks. *Proceedings of the National Academy of Sciences,* Volume 89, pp. 10915-10919.

Needleman, S. & Wunsch, C. D., 1970. A general method applicable to the search for similarities in the amino acid sequence of two proteins. *Journal of Molecular Biology,* Volume 48, pp. 443-453.