# PyMOL 2.5の インストール法

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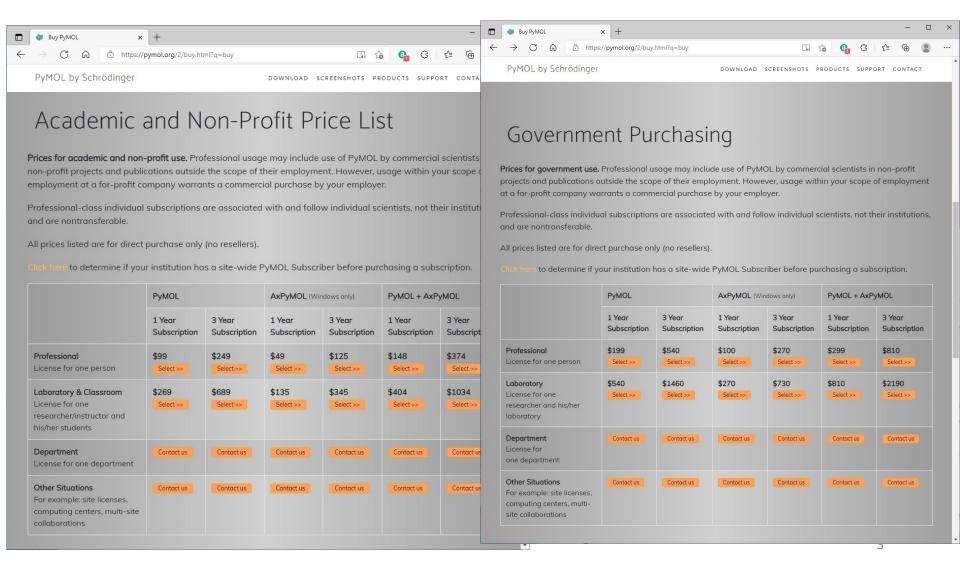
2021/08/03

# PyMOL2.5の配布法・ライセンスの種類

PyMOLは、オープンソースの分子ビューアソフトで、現在はSchrödinger社によって開発・管理が行われています。配布には、オープンソース版とIncentive PyMOLに分かれています。Incentive PyMOLにはいくつかのライセンスの種類があります。

	•		
配布法	ライセンス	費用	説明
オープンソース		無料	機能制限あり。ソースのみ無料配布のため、自分でコンパイルするか、コンパイル済みバイナリを公開している第3者のサイトからダウンロードする必要。
incentive	ライセンスなし	無料	機能制限あり。30日間の限定 使用。"No License File"の表示
今回の講習会用だけ	Commercial	要問合せ	
の使用なら、 「ライセンスなし」 か	Government	\$199/1人, 年	
「Student/Teacher」 ライセンスを 使ってください	Academic/Non-profit	\$99/1人 <i>,</i> 年	
	Student/Teacher	無料	機能制限あり。"Educational

# 本気で研究に使う場合は、 ライセンスの購入を推奨いたします



### 『有償ライセンスIncentive版とそれ以外の機能の違い

### Pylviol Product Companson Matrix

вич РуМОL

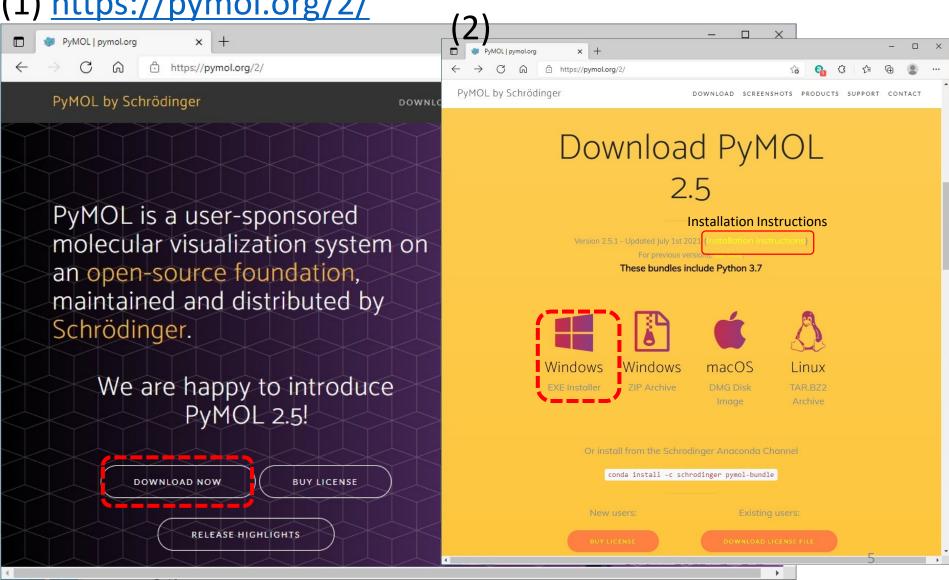
Expand Tabs below by clicking them. Compare fewer products by clicking the "Remove" box above any product on the right.	Incentive PyMOL	Open- Source PyMOL
Price		
Paid License Required	•	
Support		
Phone and Email Support	•	
Incentive Documentation and Tutorials	•	
Narrated Screencast	•	
System Integration		
Compiled and Ready to Use (Windows, Mac, Linux)	•	
Looking Glass Support	•	
3D Space Navigator Support	•	
conda package manager	•	
Scientific Integration	<i>)</i>	
Pi-Pi and Pi-Cation interactions	•	
WaterMap Result Presets	•	
MTZ Map Reading	•	
Stereochemical Determination and Labeling (PyMOL 1.x)	•	
Advanced Molecular Morphing Wizard with RigiMOL	•	
APBS Integration	•	
Direct MPEG/QuickTime export	•	
MMFF94 Forcefield	•	
Graphics		
Real-time Antialiasing	•	
Volume Visualization	•	•

Pi-Pi and Pi-Cation interactions	•	
WaterMap Result Presets	•	
MTZ Map Reading	•	
Stereochemical Determination and Labeling (PyMOL 1.x)	•	
Advanced Molecular Morphing Wizard with RigiMOL	•	
APBS Integration	•	
Direct MPEG/QuickTime export	•	
MMFF94 Forcefield	•	
Graphics		
Real-time Antialiasing	•	/a
Volume Visualization	•	•
Volume Visualization (pre-integrated)	•	
Advanced labels and callouts	•	•
Focal blur	•	
Usability		
Multilevel Undo for Building	•	
Annotated Settings	•	
New Plugin/Script Manager	•	•
CTRL-F to find objects/selections	•	
Maestro and MOE file reading support	•	
VRML and COLLADA geometry export	•	•

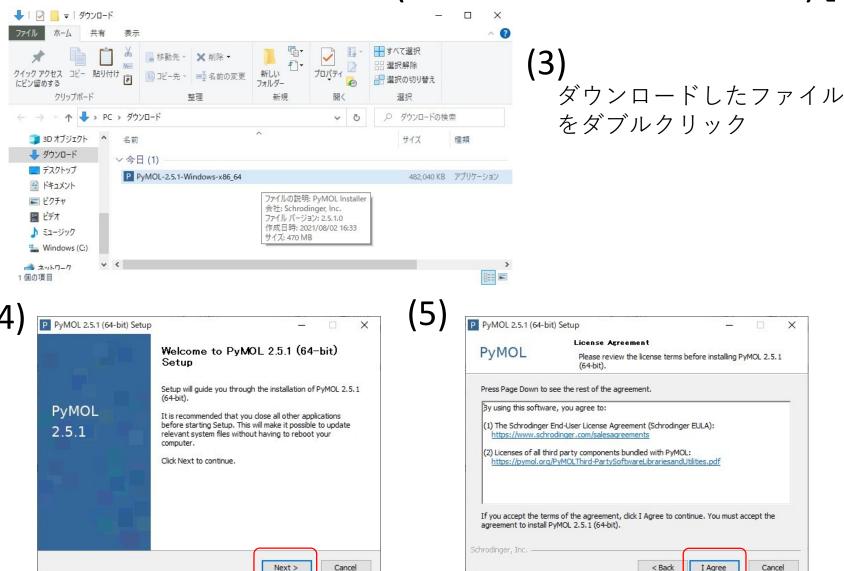
※今回の講習会では、有償ライセンス Incentive版だけの機能は使いません。

# インストール(Windowsの場合) [1]

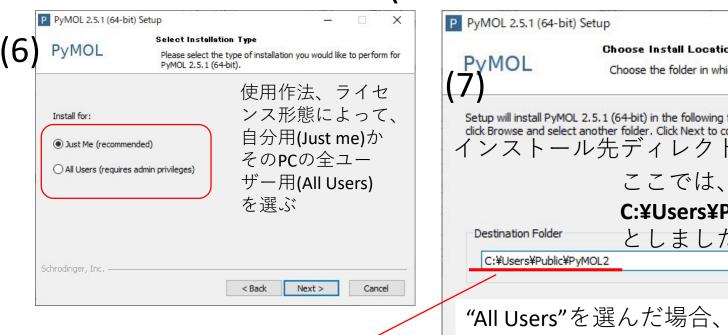
(1) https://pymol.org/2/

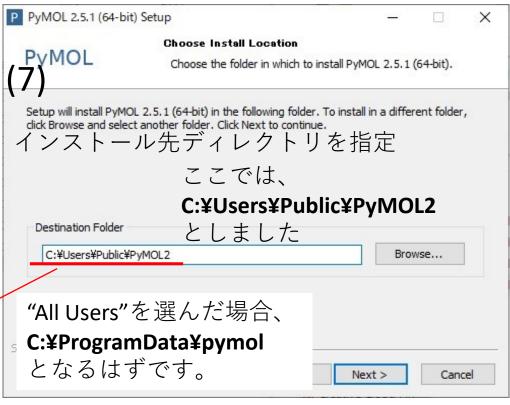


# インストール(Windowsの場合)[2]



# インストール(Windowsの場合)[3]





P PyMOL 2.5.1 (64-bit) Setup

- ※注意:インストール先のフォルダ名に
- (1) 漢字などの全角文字が入っているとエラー

"Just Me"のデフォルトは

C:¥Users¥川端 猛¥AppData¥Local¥Schrodinger¥PyMOL2 →エラー

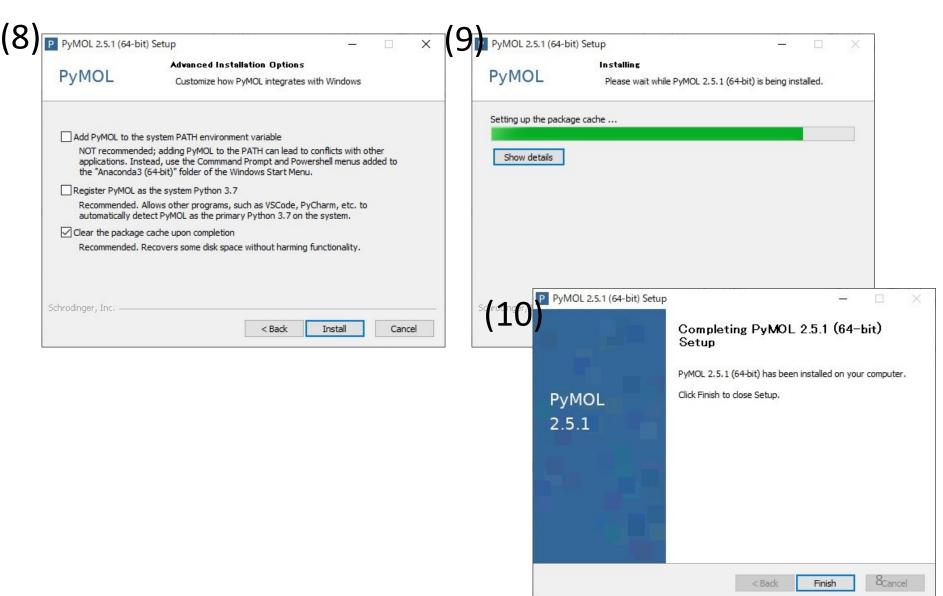
(2) フォルダ名が長すぎる(46文字以上)とエラー

C:¥Users¥Public¥AppData¥Local¥Schrodinger¥PyMOL2 → <sup>→</sup> <sup>→</sup> <sup>→</sup> <sup>→</sup> <sup>−</sup>



'Destination Folder' cannot contain non-ascii characters (special characters or diacritics). Please choose another location.

# インストール(Windowsの場合)[4]





### 他の環境の場合のインストール

# PyMOL Installation 以下のページを参考にしてください。

https://pymol.org/2/support.html?#installation

#### On Windows

- . Interactive: Execute the .exe installer and follow the setup wizard
- Non-interactive (alternative): Equivalent to Miniconda installer

  start /wait "" PyMOL-2.3.4\_0-Windows-x86\_64.exe /InstallationType=AllUsers /S /D=C:\Programs\PyMOL
- · ZIP Archive: Unzip and run PyMOLWin.exe (does not create start menu entries)

#### On a Mac

- 1. Double-click on \*.dmg file
- 2. Drag PyMOL icon to Applications folder

#### On Linux

- 1. Unpack the .tar.bz2 file, e.g.: tar -jxf PyMOL-2.2.0\_0-Linux-x86\_64.tar.bz2
- 2. Run PyMOL with: cd pymol; ./pymol

### With existing Anaconda installation

 For PyMOL 2.5: Transition from previous versions may not work. All dependencies, including python, are based off of conda-forge. More information

conda install -c schrodinger -c conda-forge pymol

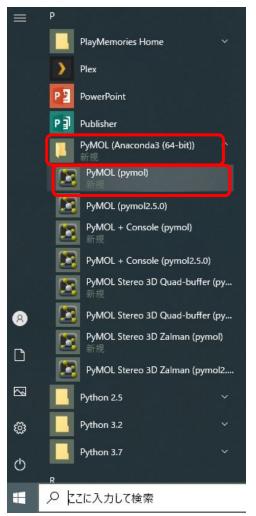
- For PyMOL 2.4 and older:
   conda install -c schrodinger pymol
- · Hint: Conda works great with isolated environments

#### License installation

• Download the license file. Save it on your workstation and then navigate to it when PyMOL prompts you for a license.

# PyMOLの起動

(1)スタートメニューからPyMOL(pymol)を選ぶ



(2) SKIP ACTIVATION 企業 S

Activation ? ×

Activation

You are running an official PyMOL build ("Incentive PyMOL") from Schrödinger, Inc, which requires a subscription-based license. To obtain a license, visit https://pymolorg/buy

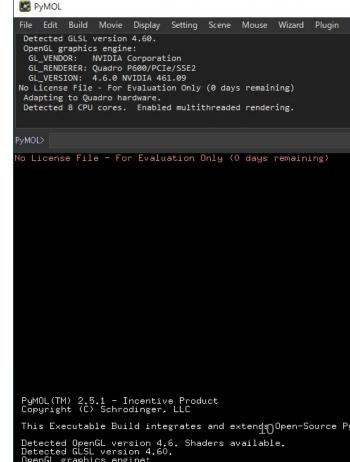
Browse for License File

You may evaluate PyMOL for a period of 30 days. A "No License File" notice will appear in the graphics window when the evaluation period has ended, and the morphing feature will be disabled.

Skip Activation

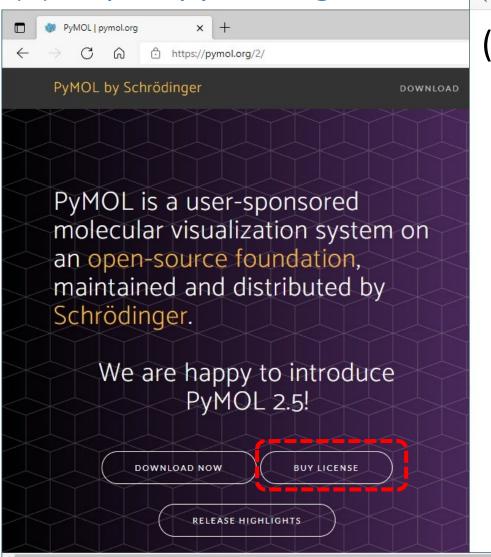
※ただし、機能限定版。使用日数の制限もあり。また、画面に常に"No License File"と表示される。

(2) Skip Activationを選ぶ (3) 「ライセンスなし」 \*\*\*\* のPyMOLが起動



### ライセンスの取得: Student/Teacherの場合[1]

### (1) <a href="https://pymol.org/2/">https://pymol.org/2/</a>



# C の https://pymol.org/2/buy.html?q=buy PyMOL by Schrödinger Student/Teacher を表します。 Student/Teacher を表しまする。 Student/Teacher を表します。 Student/Teacher を表します。 Student/Teacher を表します。 Student/Teacher を表します。 Student/T

### Buy PyMOL

Buy PyMOL

Order PyMOL and AxPyMOL Online

Please select your intended use from the list below to receive access within one business

- Commercial Commercial for corporate organizations
- Government Government for government institutions
- Academic/Non-profit
   Academic/Non-profit

for academic and non-profit researchers/educators

### Student/Teacher Student/Teacher

Educational subscriptions to PyMOL are available at no cost to full-time students are full-time students. However, there is not an educational subscription for AxPyMOL agreement, Schrödinger has no obligation to furnish updates, fix bugs, provide docuother support needs. Please recognize that long-term reliance upon PyMOL for educational merit a subscription purchase in order to secure essential services and basel

All paid subscriptions include software upgrades for the duration of the subscription term and access to Official Online Documentation.

### ライセンスの取得: Student/Teacherの場合[2]

### (3a) "Teacher"の場合の記入例

## Registration For Educational-Use-Only PyMOL Builds

Schrödinger offers **Educational-use-only** PyMOL builds available at no cost to **teachers and high school and college students** (including online courses, homeschooling, etc.) for classroom

-> FAQ (Frequently Asked Questions)

instruction, homework assignments, and to provide a means for creating high quality figures. Please note that it is not provided for the purposes of academic research or publication.

The Educational-use-only PyMOL builds are provided "AS IS" with no obligation to grant download access, fix bugs, furnish updates, provide documentation, or meet any other need related to the educational-use PyMOL builds.

If you intend to use PyMOL products for academic research or publication, please purchase an Academic PyMOL subscription, which includes access to technical support, screencasts, and additional resources. See <a href="http://pymol.org/academic">http://pymol.org/academic</a>.

I am a:	Teacher 🕶	
Your First Name:	Takeshi	
Your Last Name:	Kawabata	
Your Email Address:	kawabata@protein.osaka-u.a	
Your Telephone Number:	81727294155	
Institution:	Osaka University	
Comments (optional):		
Class Name:	Advanced Research:CryoEN	担当している講義の名前
Class Number:	241763	講義番号
Class Duration (through date):	2021	講義期間
Continue		

### ライセンスの取得: Student/Teacherの場合[3]

### (3b) "Student"の場合の記入例

### Registration For Educational-Use-Only PyMOL Builds

Schrödinger offers **Educational-use-only** PyMOL builds available at no cost to **teachers and high school and college students** (including online courses, homeschooling, etc.) for classroom

-> <u>FAQ (Frequently Asked Questions)</u>

instruction, homework assignments, and to provide a means for creating high quality figures. Please note that it is not provided for the purposes of academic research or publication.

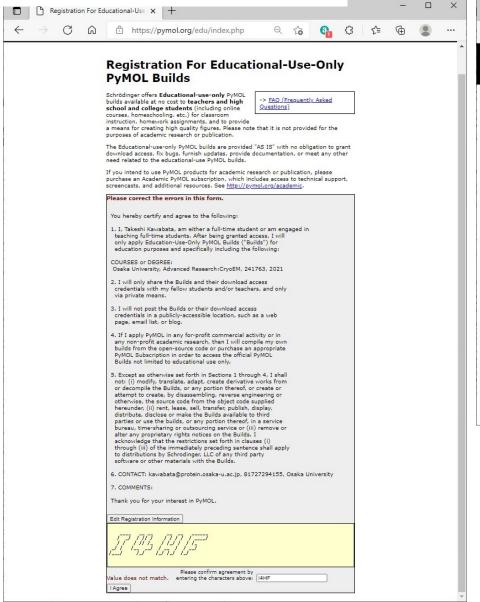
The Educational-use-only PyMOL builds are provided "AS IS" with no obligation to grant download access, fix bugs, furnish updates, provide documentation, or meet any other need related to the educational-use PyMOL builds.

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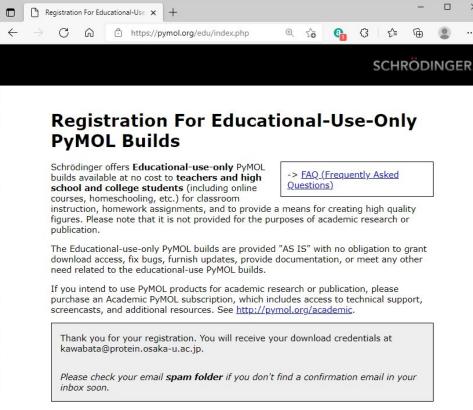
I am a: [	Student 🗸
Your First Name:	Takeshi
Your Last Name:	Kawabata
Your Email Address:	kawabata@protein.osaka-
Your Telephone Number:	+81727294155
Institution:	Osaka University
Comments (optional):	
Degree:	PhD <b>v</b> 学士、修士、博士などの区別
Subject Matter:	Structural Bioinformatics 研究分野
Name of Your Advisor or Instructor:	Genji Kurisu 指導教員
Anticipated Award Year:	2022 🕶 取得予定年
Continue	

### ライセンスの取得: Student/Teacherの場合[4]

(4) Agreementの確認



(5)



### ライセンスの取得: Student/Teacherの場合[5] (6) 電子メールの確認

差出人: help@schrodinger.com

送信日時: 2021年8月2日月曜日 17:32 宛先: kawabata@protein.osaka-u.ac.jp 件名: PyMOL Educational Use Declaration for

Takeshi Kawabata

You hereby certify and agree to the following:

1. I, Takeshi Kawabata, am either a full-time student or am engaged in teaching full-time students. After being granted access, I will only apply Education-Use-Only PyMOL Builds ("Builds") for education purposes and specifically including the following:

COURSES or DEGREE: Osaka University, Advanced Research: CryoEM, 241763, 2021

- 2. I will only share the Builds and their download access credentials with my fellow students and/or teachers, and only via private means.
- 3. I will not post the Builds or their download access credentials in a publicly-accessible location, such as a web page, email list, or blog.
- 4. If I apply PyMOL in any for-profit commercial activity or in any non-profit academic research, then I will compile my own builds from the open-source code or purchase an appropriate PyMOL Subscription in order to access the official PyMOL Builds not limited to educational use only.
- 5. Except as otherwise set forth in Sections 1 through 4, I shall not: (i) modify, translate, adapt, create derivative works from or decompile the Builds, or any portion thereof, or create or attempt to create, by disassembling, reverse engineering or otherwise, the source code from the object code supplied hereunder, (ii) rent, lease, sell, transfer, publish, display, distribute, disclose or make the Builds available to third parties or use the builds, or any portion thereof, in a service bureau, time-sharing or outsourcing service or (iii) remove or alter any proprietary rights notices on the Builds. I acknowledge that the restrictions set forth in clauses (i) through (iii) of the immediately preceding sentence shall apply to distributions by Schrodinger, LLC of any third party software or other materials with the Builds.
- 6. CONTACT: kawabata@protein.osaka-u.ac.jp, 81727294155, Osaka University
- 7. COMMENTS:

Thank you for your interest in PyMOL.

DOWNLOAD URL: https://pymol.org/ep

**USERNAME:** PASSWORD:

DOWNLOAD URL: <a href="https://pymol.org/ep">https://pymol.org/ep</a> にアクセス、送付されてきた[USERNAME]と [PASSWORD]を入力

15

### ライセンスの取得: Student/Teacherの場合[6]

(7)DOWNLOAD URL: <a href="https://pymol.org/ep">https://pymol.org/ep</a>

にアクセス、送付されてきた[USERNAME]と

[PASSWORD]を入力

ユーザー名	
パスワード	

(8) License File : pymol-edu-license lic をダウンロード

# → C A https://pymol.org/ep/ SCHRÖDINGER Download Educational-Use-Only PyMOL DO NOT SHARE THESE FILES OUTSIDE OF EDUCATIONAL ENVIRONMENTS

-- they are for students and teachers only.

To the extent that you redistribute these files or the download credentials

To the extent that you redistribute these files or the download credentials internally, please be sure that access is appropriately limited. Although primarily intended for classroom use, students, and teachers may download and use these builds on personal computers for educational tasks such as homework assignments.

#### PyMOL Executable Builds for Educational Use Only

Registration For Educational-Use X Download Educational-Use-Only X

The Educational-use-only PyMOL builds are provided "AS IS" with no obligation to grant download access, fix bugs, furnish updates, provide documentation, or meet any other need related to the educational-use PyMOL builds. Purchased <a href="PyMOL Academic Subscriptions">PyMOL Academic Subscriptions</a> with up to three years of maintenance are available to meet your longer-term educational use needs.

#### PyMOL 2.0 (September 2017)

License File: pymol-edu-license.lic

Installers: PyMOL Download Page

#### PyMOL 1.7.4 (August 2015)

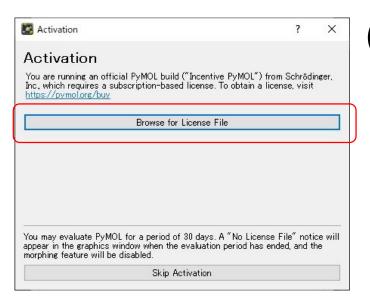
Windows 64bit: <u>EduPyMOL-v1.7.4.5-Win64.msi</u>
Windows 32bit: <u>EduPyMOL-v1.7.4.5-Win32.msi</u>

OS X 10.7+: EduPyMOL-v1.7.4.5r1.dmg

Linux 64bit: EduPvMOL-v1.7.4.5-Linux-x86 64.tar.bz2

### ライセンスの取得: Student/Teacherの場合[7]

- (8) PyMOLを再起動
- (9) [Browse for License File]をクリックし、 ダウンロードしたファイル"pymol-edu-license.lic"を指定



※ただし、機能限定版。 使用日数の制限はない。 また、画面に常に "For Educational Use Only" と表示される。

(10) 「Student/Teacher」 ライセンスの

