SASpy - ATSAS PyMOL Plugin Tutorial

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SAS EMBO Course

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Outline

- SASpy introduction
- Live demo:
  - loading and editing 3D models
  - interactive hybrid modeling
  - low- and high-res model superposition
  - tips for creating figures
- Installation and related politics
SASpy: a PyMOL Plugin for SAS hybrid-modeling

- Click-and-point interface for SAS hybrid-modeling
SASpy: integrating ATSAS and PyMOL

- **SASpy** combines **ATSAS** and **PyMOL**
- **ATSAS** SAS analysis software package
  - Freely available for academics
  - Compiled for Win, Mac and Linux
  - From initial data reduction to advanced modeling
- **PyMOL** Molecular visualization software
  - Visualize and edit 3D molecular models
  - Ray-rendering for publication quality figures
  - Extensible through ‘plugins’
SASpy live demo

- loading and editing 3D models
- interactive hybrid modeling
- low- and high-res model superposition
- tips for creating figures
PyMOL was developed by Warren DeLano and it is open source.

**Linux and Mac OS X**, straightforward and FREE installation:
- Linux: `sudo apt-get install pymol` (also rpm, yum, etc)
- Mac OS X: `brew install pymol` (also fink or macports)

Compile it yourself: sourceforge.net/projects/pymol/
PyMOL installation (Windows)

- Still open source, just not easy to compile on Windows...
- Alternative: binaries distributed by Schrödinger LLC:
  - Free educational version: pymol.org/edu/?q=educational/
  - Edu version is only useful for Windows SASpy, it won’t work properly on OS X or Linux
  - Academics version at pymol.org/academic 99 $ per year
- For the brave Windows expert, please try to compile it and let us know
  pymolwiki.org/index.php/Windows_Install
Install SASpy as a PyMOL plugin

1. Open PyMOL
2. Go to menu: Plugin, Plugin Manager, Install New Plugin
3. Navigate to the `saspy.py` file
   - Linux: `/usr/share/atsas/pymolplugin`
   - OS X: `/Applications/ATSAS/share/pymolplugin`
   - Windows: `C:\atsas\share\pymolplugin`
   - Cross-platform, just grab it from GitHub: `github.com/emblsaxs/saspy`
4. Say YES to the questions that may popup
5. Restart PyMOL and SASpy should be available at the Plugin menu
Thanks for your attention!

- Questions?
- Complaints?
- Ideas?
- Please contact us (email to: atsas@embl-hamburg.de)
- There’s a reference for SASpy:
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