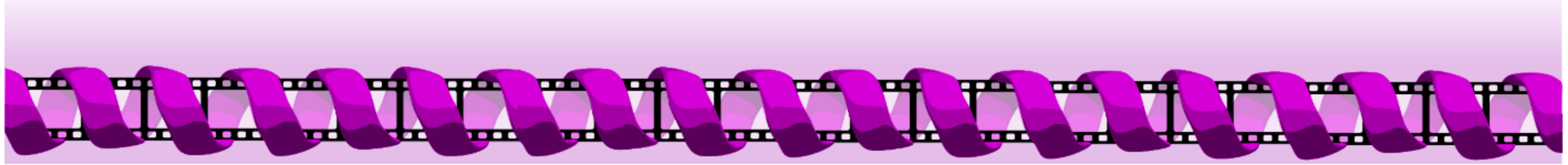
Molecular movies made easy with

MOLYWOOD

BioExcel webinar
22.10.2020

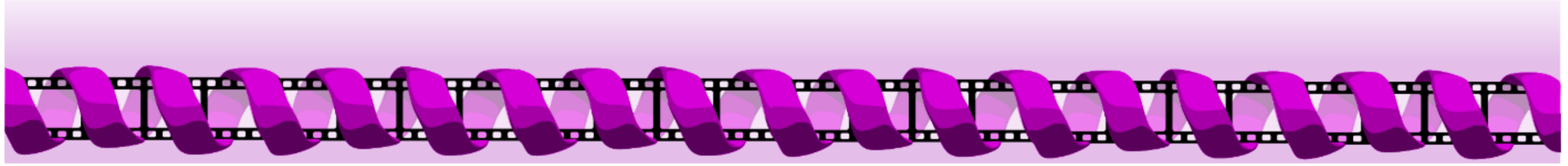
Miłosz Wieczór
Molecular Modelling and Bioinformatics, IRB Barcelona
Dept of Physical Chemistry, Gdansk University of Technology



The background story

- Born out of a sense of common frustration
- Few tools available, mostly Python or Tcl libraries
- Either simplistic or complex: a big gap in between
- Simple syntax & extensive documentation
- Two guiding principles:

1. make it 'plug-and-play'
2. keep easy things easy, complex things doable



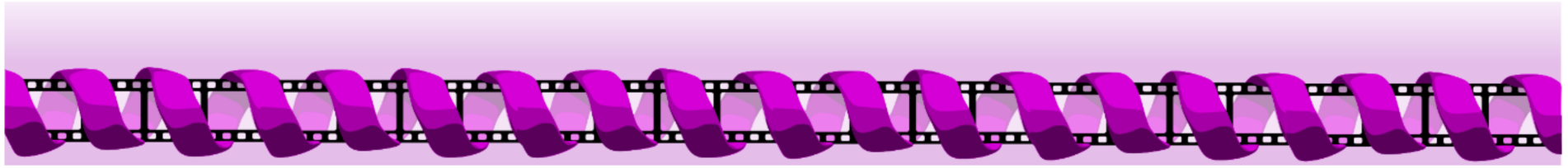
The background story 2

Users: computational biologists at all levels of expertise

Goal: push for a broader recognition of movies as a tool for dissemination

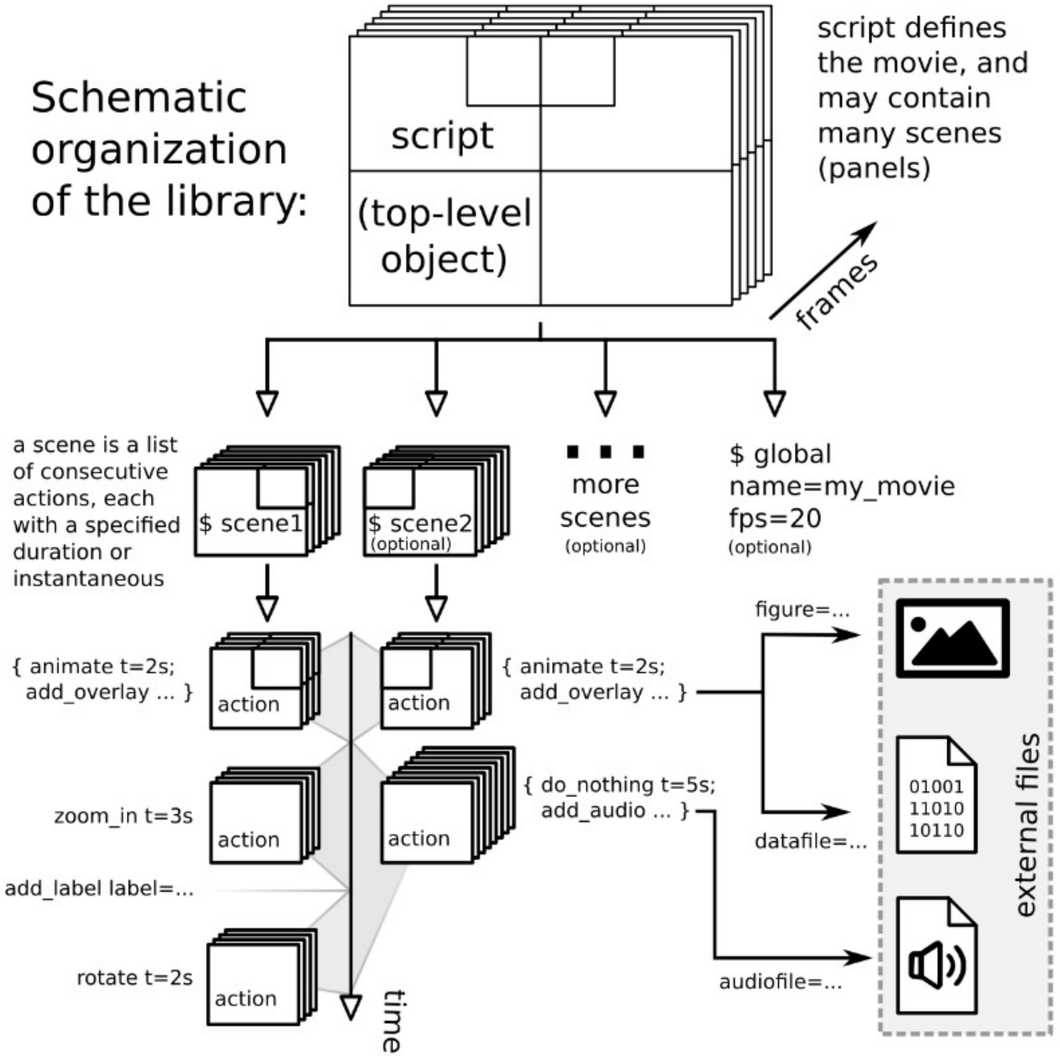
Means: make movie design fun

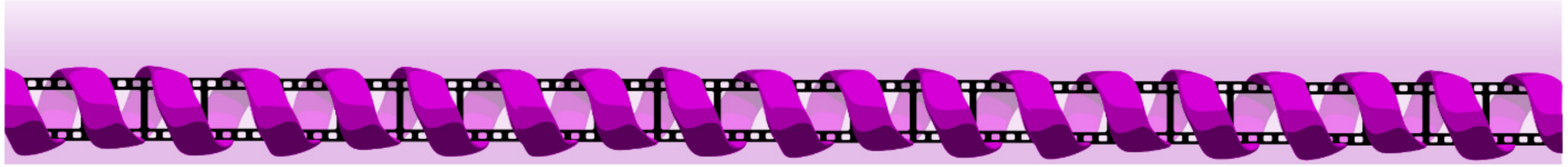
Structure: as modular and flexible as possible to foster creativity



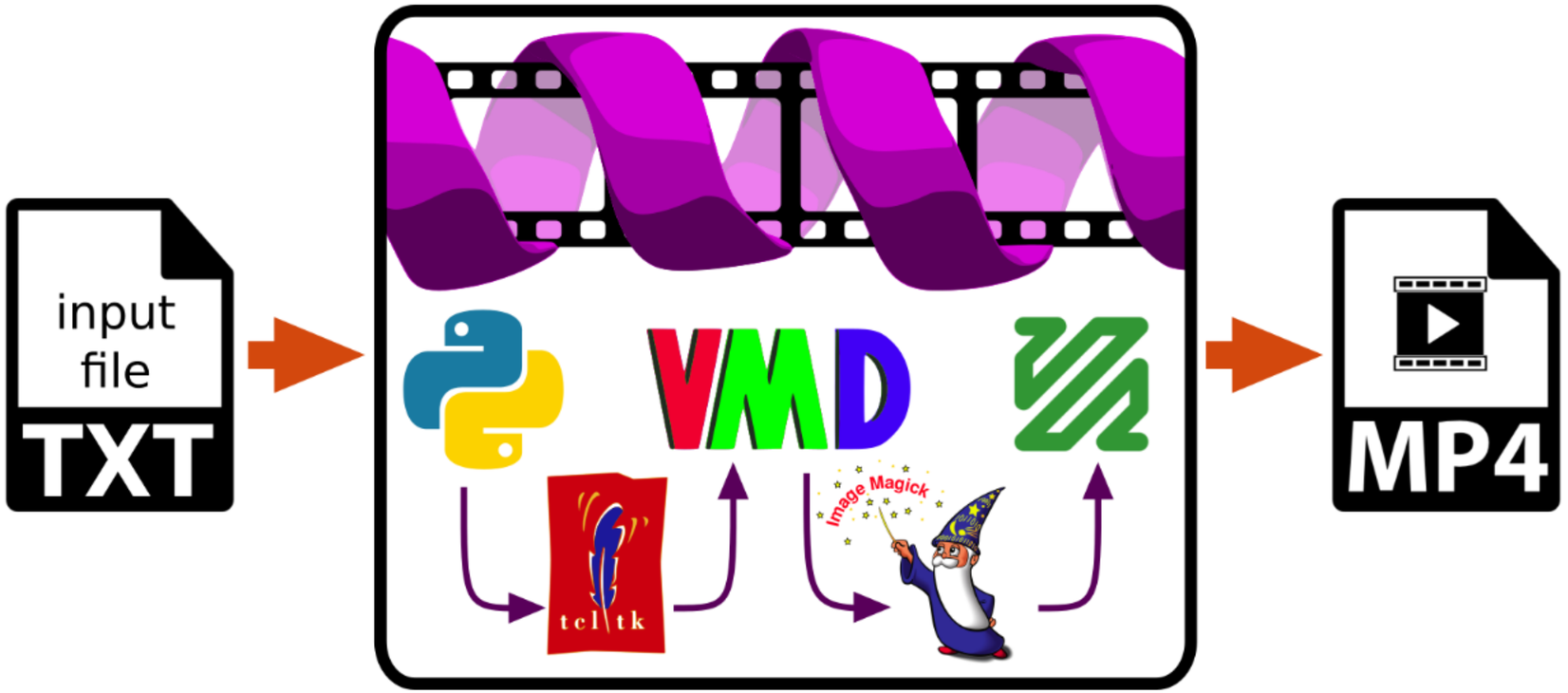
Tool structure

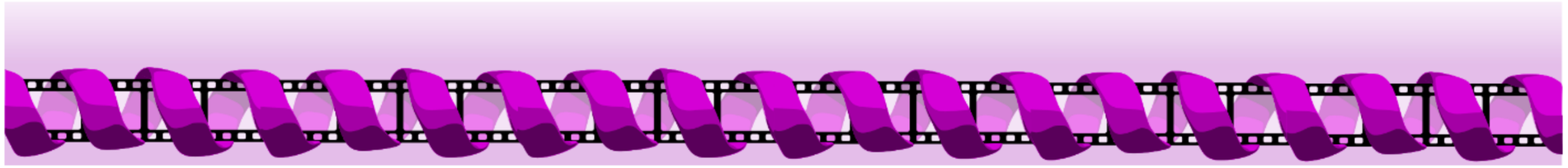
Schematic organization of the library:





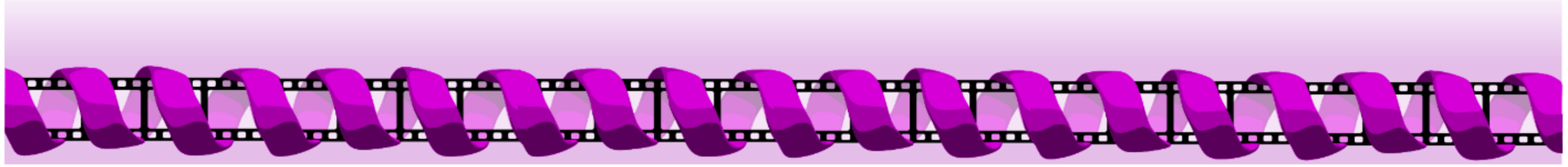
What's under the hood





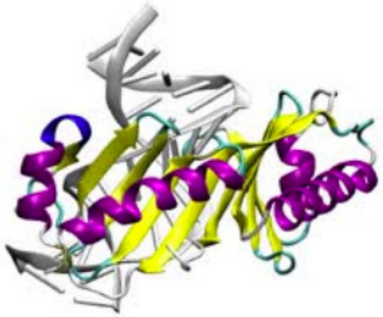
Easy installation

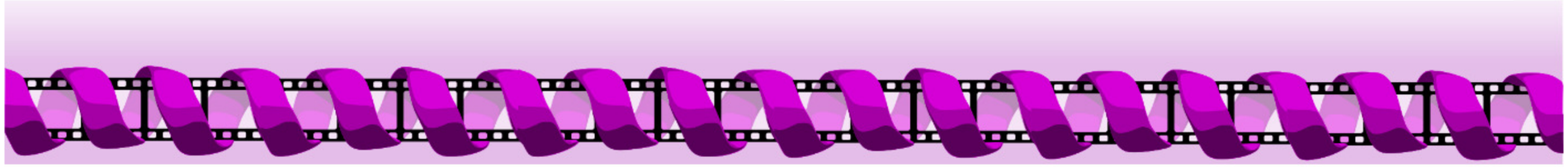
- Have ffmpeg, VMD and python/numpy? Just go for pip install molywood
- Safer version: through CONDA (see tutorials)
    1. modify existing venv
    2. create a new venv molywood
- Type molywood-gen-env to check and setup, and molywood to run
- Tested on Windows, Linux and Mac



A minimal example

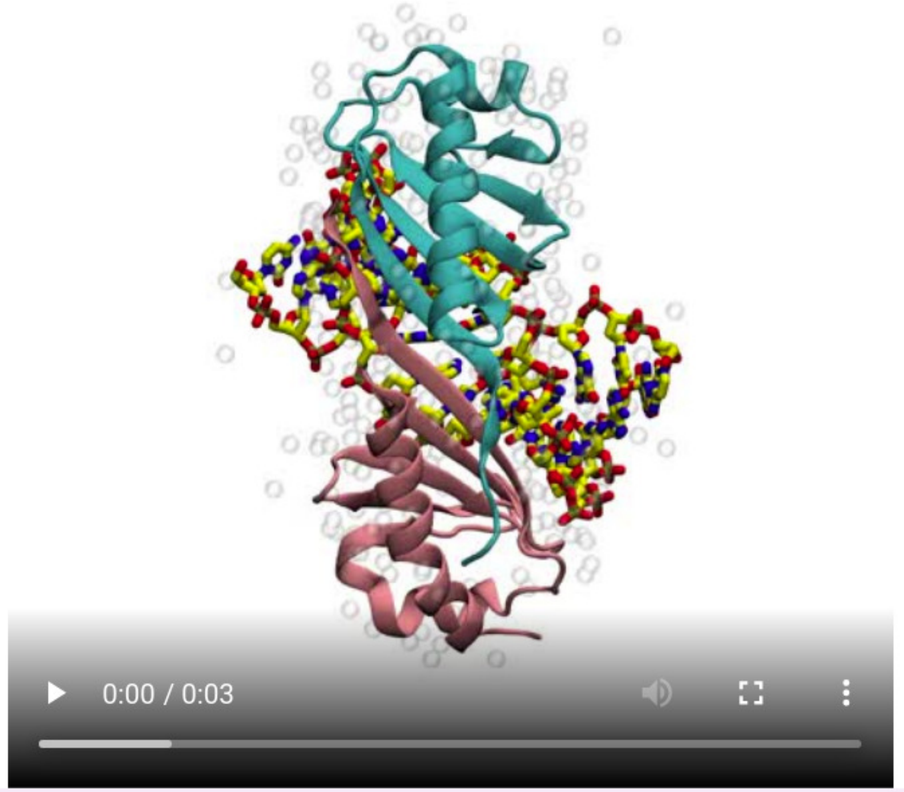
```
$ global name=movie1
$ scene_tbp pdb_code=1cdw

# scene_tbp
zoom_in  scale=1.4 t=2s
rotate   axis=y angle=360 t=2s
```

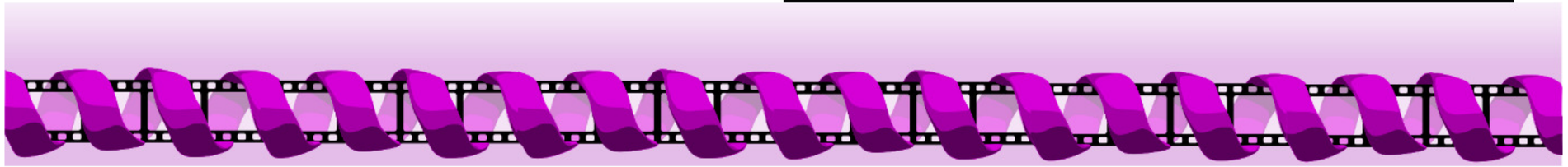




Custom representations

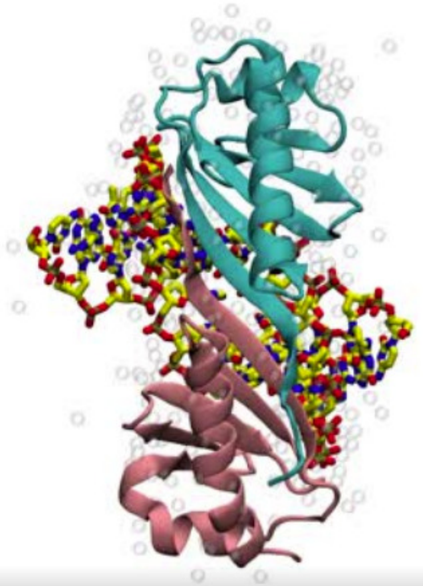
```
$ global name=movie2
$ scene_tbp visualization=cust.vmd

# scene_tbp
zoom_in  scale=1.4 t=2s
rotate   axis=y angle=360 t=2s
```

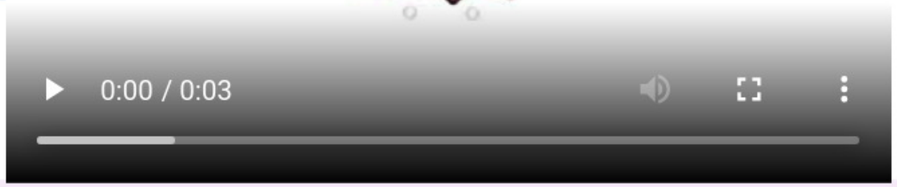


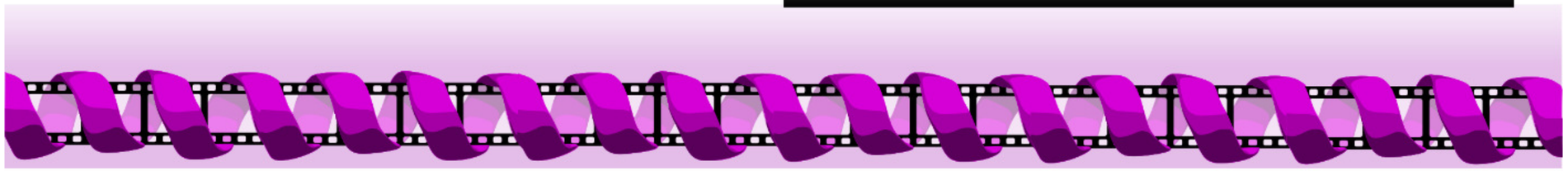


...or made from scratch

```
$ global name=movie3
$ scene_tbp pdb_code=1cdw

# scene_tbp
rotate axis=z angle=75
zoom_in scale=1.2
make_transparent material=opaque

highlight selection='nucleic and noh'
 style=licorice color=type thickness=1.5 mode=u
 material=diffuse
highlight selection='protein and resid < 247'
 style=newcartoon color=10 mode=u material=diffuse
highlight selection='protein and resid > 247'
 style=newcartoon color=9 mode=u material=diffuse
highlight selection=water style=vdw
 thickness=0.5 mode=u alpha=0.1

zoom_in  scale=1.4 t=2s
rotate   axis=y angle=360 t=2s
```

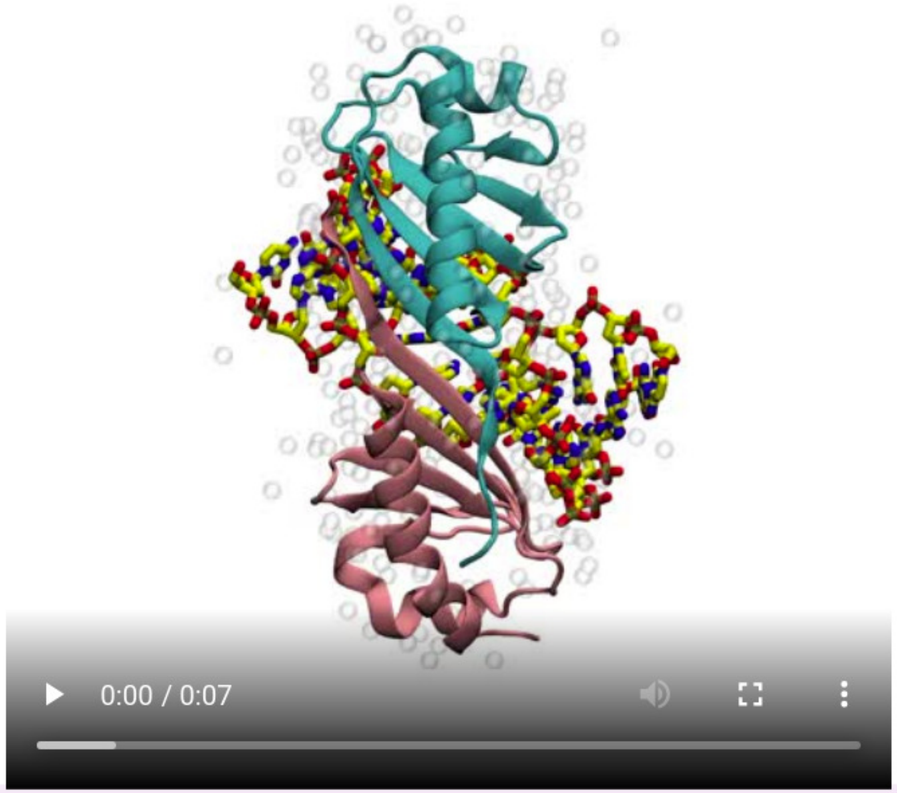


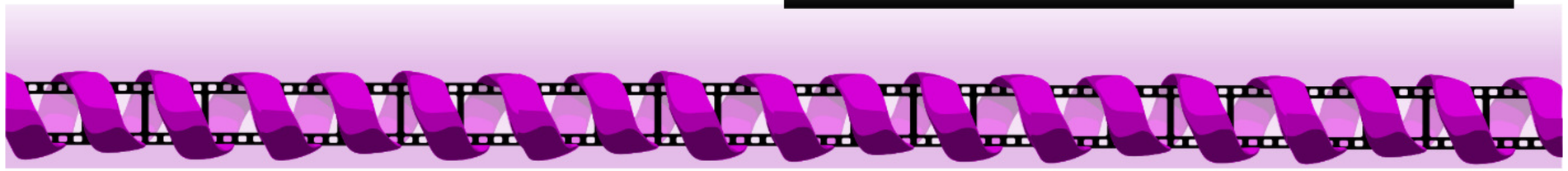




Instantaneous or finite-time

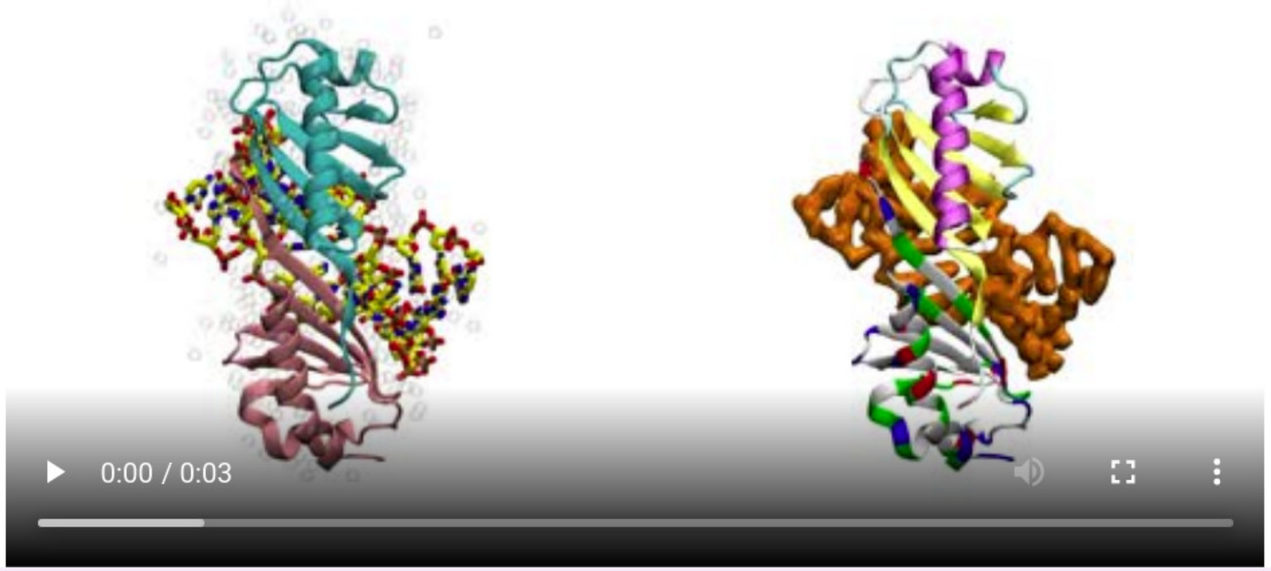
```
$ global name=movie4
$ scene_tbp pdb_code=1cdw

# scene_tbp
zoom_in    scale=1.4 t=2s
rotate     axis=y angle=15
zoom_out   scale=1.4 t=2s
translate vector=0,0.2,0
rotate     axis=y angle=120 t=2s
fit_trajectory selection=nucleic
axis=z
highlight selection='resname LYS'
 style=vdw color=element mode=u
 material=diffuse
rotate     axis=y angle=-120 t=2s
```

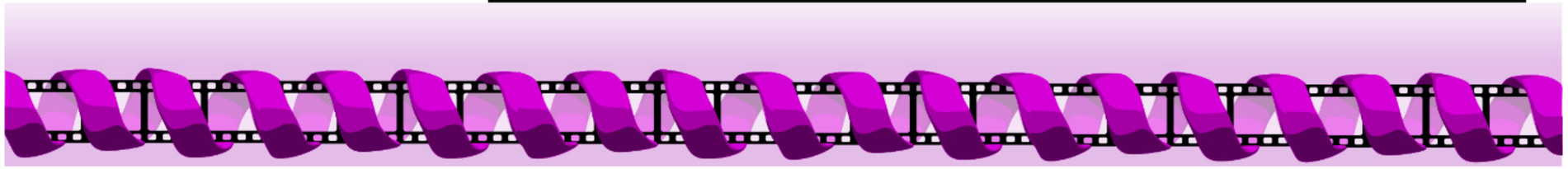




A grid of Scenes

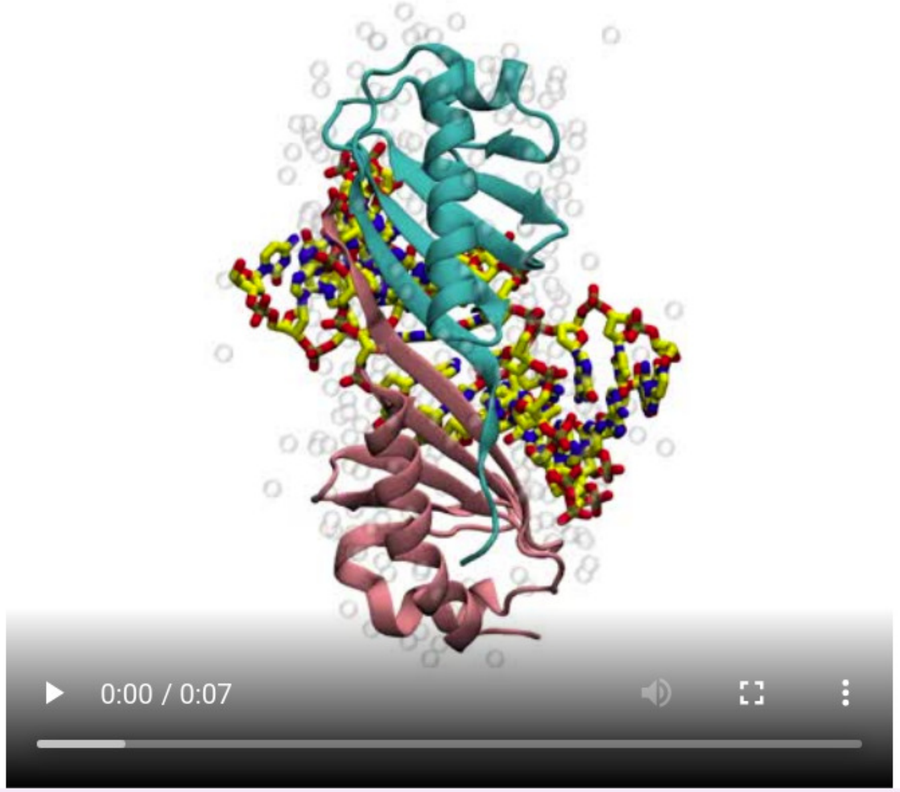
```
$ global name=movie5
$ layout rows=1 columns=2
$ sc1 visualization=custom1.vmd position=0,0
$ sc2 visualization=custom2.vmd position=0,1

# sc1,sc2
zoom in scale=1.4
  t=2s
rotate axis=y
  angle=360 t=2s
```

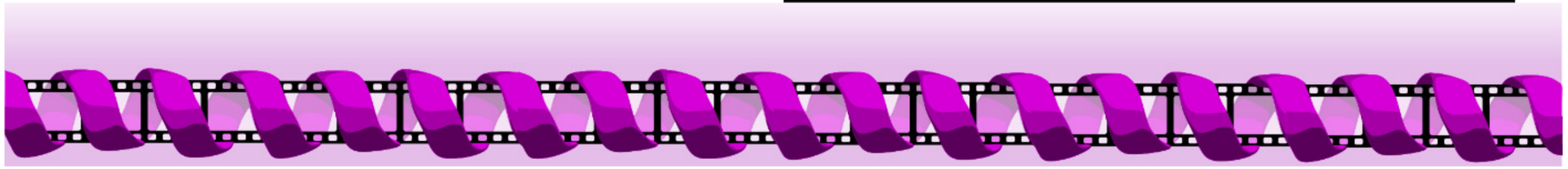




A sequence of Scenes

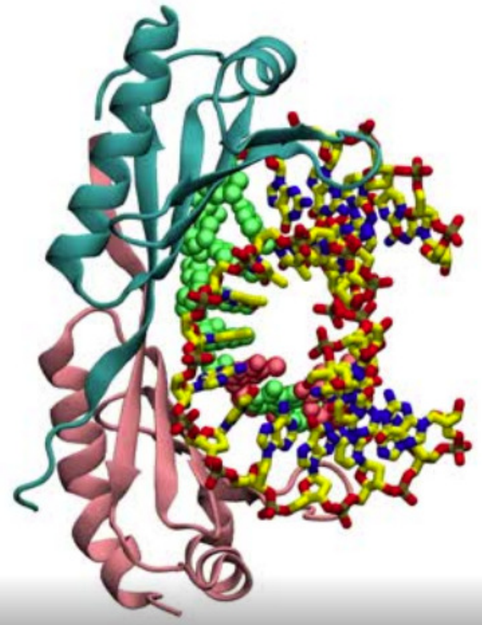
```
$ global name=movie6
$ sc1 visualization=custom1.vmd
$ sc2 visualization=custom2.vmd
  after=sc1

# sc1,sc2
zoom in scale=1.4
  t=2s
rotate axis=y
  angle=360 t=2s
```

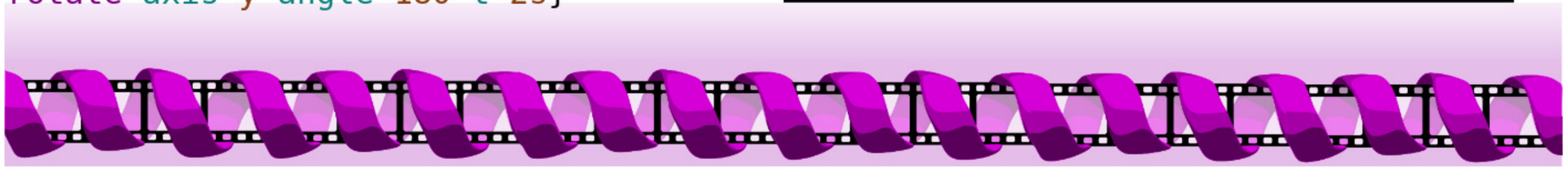




Overlays with text & images

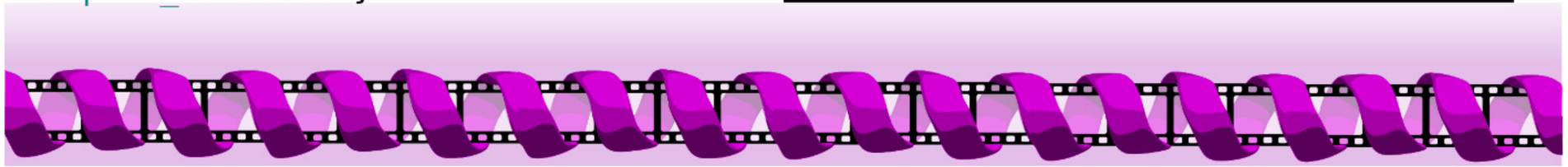
```
$ global name=movie7
$ scene_tbp visualization=cu.vmd

# scene_tbp
zoom_in scale=1.4 t=2s
{add_overlay figure=logo.png
  origin=0,0.8 transparent_background=t
  relative_size=0.4;
rotate axis=y angle=-180 t=2s}
{add_overlay figure=logo.png
  origin=0,0.8 transparent_background=t
  relative_size=0.4;
do_nothing t=2s}
{add_overlay text=consensus:
  origin=0.02,0.93;
add_overlay text=TATAAAA
  origin=0.02,0.85;
rotate axis=y angle=180 t=2s}
```





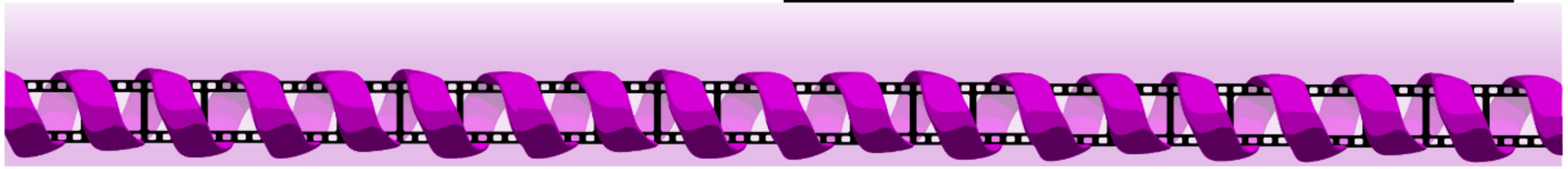
Overlays with data

```
$ global name=movie8
$ scene_tbp visualization=cu.vmd

# scene_tbp
animate frames=150
fit_trajectory selection=protein
rotate axis=y angle=-90
rotate axis=y angle=90 t=2s

{animate frames=150:750 smooth=5 t=5s;
add_overlay datafile=data.txt
  origin=0,0.6 relative_size=0.4
  aspect_ratio=0.6}
do_nothing t=1s
{animate frames=750:150 smooth=5 t=5s;
add_overlay datafile=data2.txt
  origin=0,0.6 relative_size=0.4
  aspect_ratio=0.6}
```



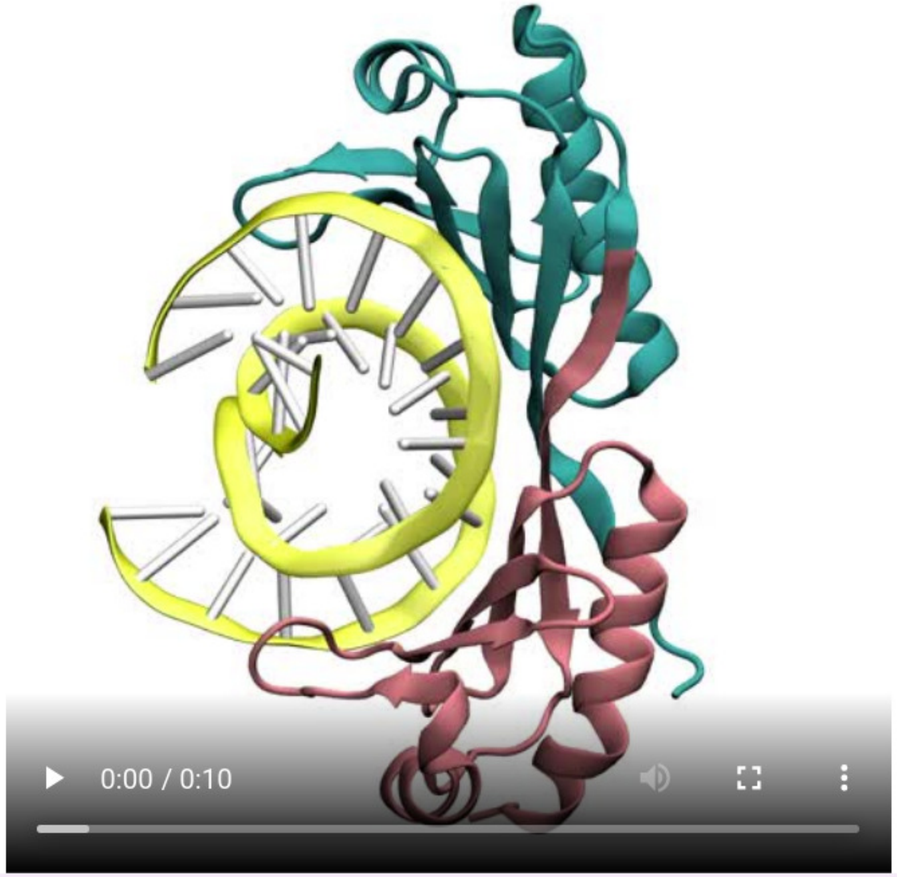
Scenes as overlays

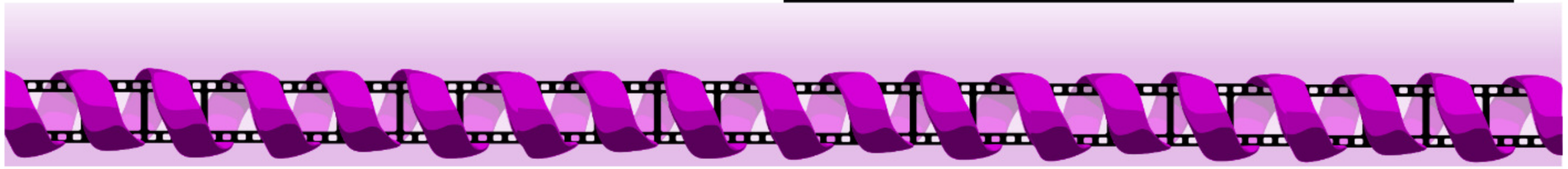
```
$ global name=movie9
$ scene_tbp visualization=cu.vmd
$ sco1 visualization=cu.vmd

# scene_tbp,sco1
animate frames=150
fit_trajectory selection=protein
rotate axis=y angle=-90

# scene_tbp
rotate axis=y angle=90 t=2s
{do_nothing t=1s;
add_overlay scene=sco1 transparent_background=t
  mode=u origin=0,0:0.65 relative_size=1:0.4}
animate frames=150:750 smooth=5 t=5s
do_nothing t=1s
animate frames=750:150 smooth=5 t=5s

# sco1
rotate axis=y angle=90
make_transparent material=Diffuse
do_nothing t=1s
animate frames=150:750 smooth=5 t=5s
do_nothing t=1s
animate frames=750:150 smooth=5 t=5s
```



On-the-fly highlight edits

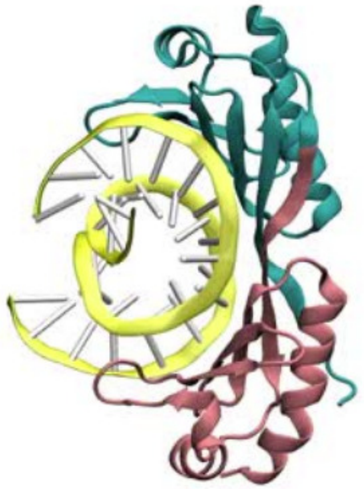
```
$ global name=movie10
$ scene_tbp visualization=cu.vmd

#scene_tbp
do_nothing t=1s
highlight selection='same residue as
(resname LYS ARG and within 5 of
nucleic)' style=licorice mode=u
color=type t=1s alias=sc fade_in=1.0
{rotate axis=y angle=360 t=3s
fraction=:0.5;
highlight alias=sc mode=n thickness=1:3}
{rotate axis=y angle=360 t=3s
fraction=0.5:;
highlight alias=sc mode=n thickness=3:1}
highlight alias=sc mode=d t=2s
do_nothing t=1s
```

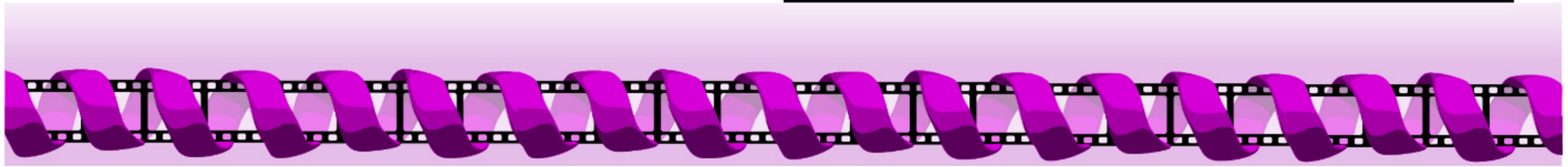


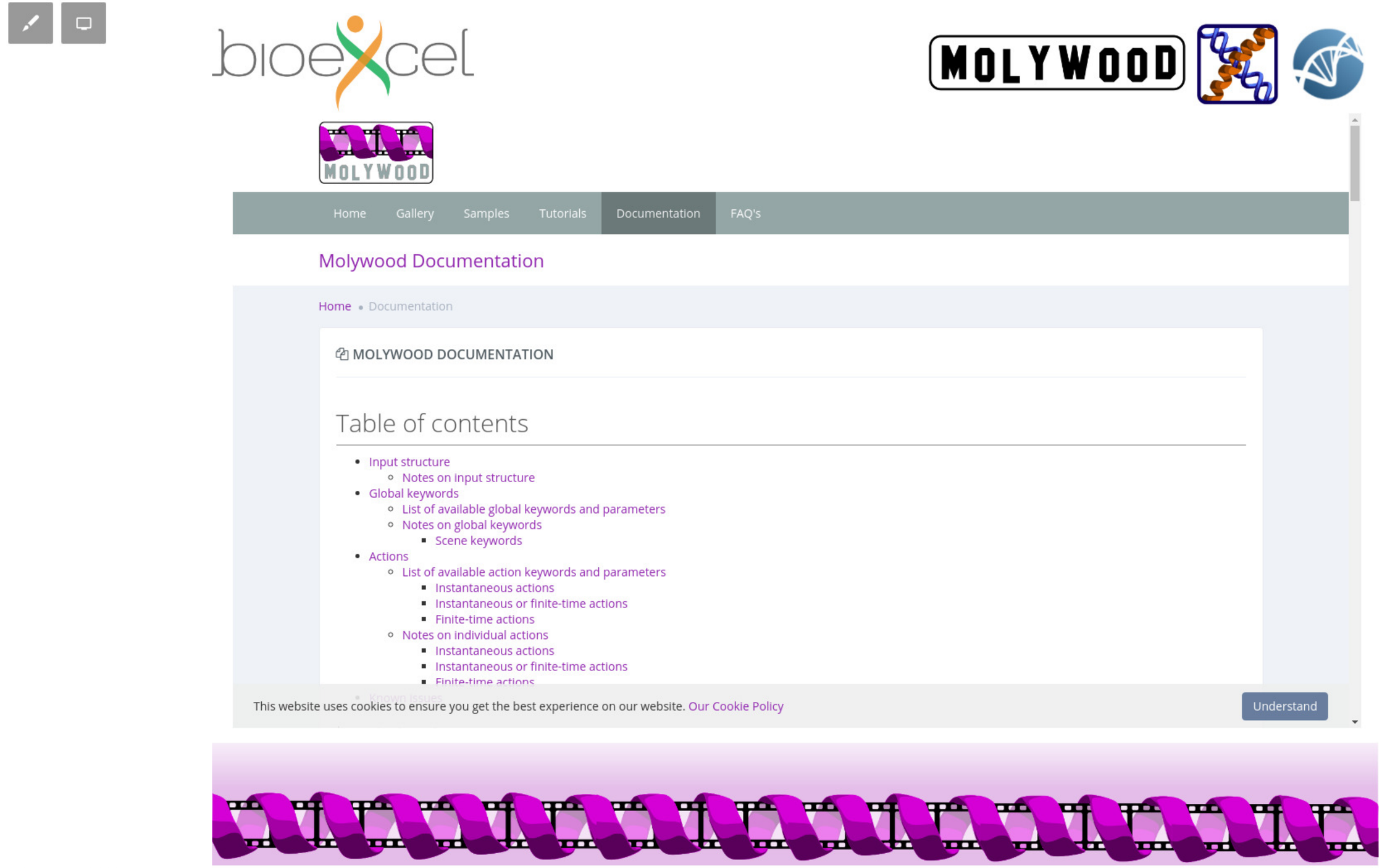


Overlapping actions

```
$ global name=movie11
$ scene_tbp visualization=cu.vmd

#scene_tbp
zoom_in scale=1.5 fraction=:0.5 t=2s
{rotate axis=y angle=360
  fraction=:0.5 t=2s;
zoom_in scale=1.5 fraction=0.5:}
{rotate axis=y angle=360
  fraction=0.5: t=2s;
translate vector=2.4,0,0
  fraction=0:0.5}
translate vector=-2.4,0,0
translate vector=2.4,0,0
fraction=0.5: t=2s
```







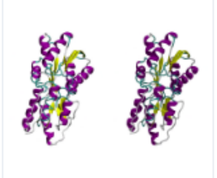
Home Gallery Samples Tutorials Documentation FAQ's

Molywood samples

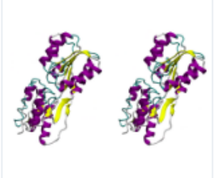
Home • Samples

BASIC OPTIONS

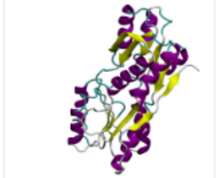
basic1



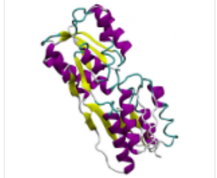
render1



render2

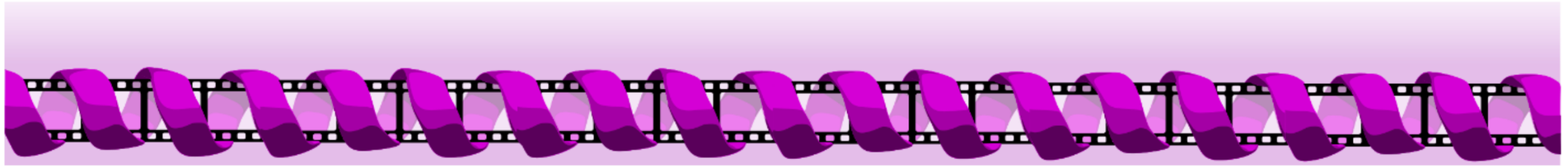


audio1



audio2

CAMERA OPTIONS

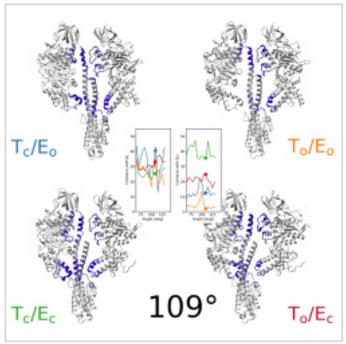


Home Gallery Samples Tutorials Documentation FAQ's

Molywood movies gallery

Home • Gallery

γ-β^{E} AND γ-β^{TP} CONTACTS IN DIFFERENT F1-ATP SYNTHASE CONFORMATIONAL STATES



Rotation of the F1-ATP synthase γ subunit in all possible conformational states of β^{TP} (T, blue) and β^{E} (E, red). As the catalytic subunits assume an open or closed geometry, they maintain different number of contacts with the central γ subunit during the two shorter (25 and 30 degree) rotary substeps, moving from 65 to 120 degrees in the synthesis direction. The plots show γ-β^{E} and γ-β^{TP} contacts, and color-coding maps the contact frequency onto the structure of the enzyme.

Open gallery example </> Open code example

D-RIBOSE BINDING PROTEIN CONFORMATIONAL TRANSITION

Movie design workflow:

Explore

```
render=f draft=t
 t=1s
```

Tweak

```
render=t draft=t
fps=2
place overlays at
low resolution
```

Adjust

```
render=t draft=t
fps=5
adjust timing
```

Test

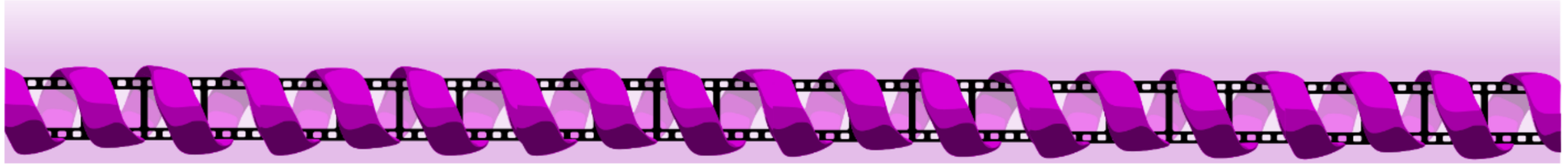
```
render=t draft=t
fps=15
set final resolution
```

Full render

```
render=t draft=f
fps=25
wait a few minutes
```

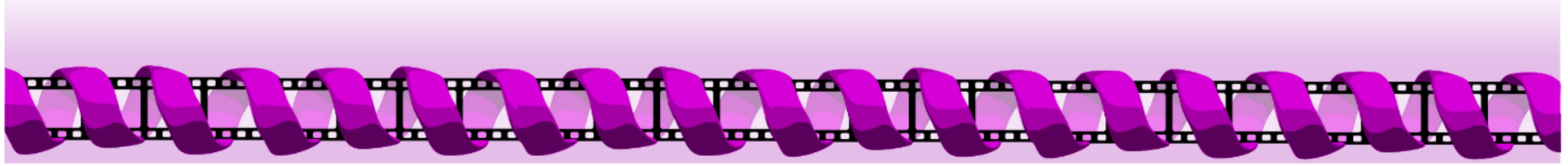
Go HQ

```
render=t draft=f
fps=25
ambient_occlusion=t
```



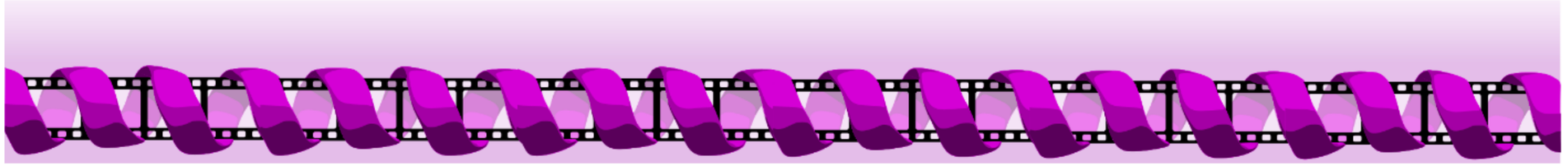
Key features, summarized

- From .txt to .mp4 with no extra requirements
- Ease of working with data, graphics, audio, movies
- Support for concurrent and/or asynchronous actions
- Flexibility in the treatment of scenes
- Highly customizable & dynamic representations
- Can be automated and run remotely
- Open and free



Future developments

- Now entirely dependent on your feedback
- Add more actions?
- Enable editing of defaults?
- Support anything beyond VMD?
- GUI or TUI-only?
- Ongoing debugging
- Gallery open to your examples



Thanks for your attention!

Now, go check out more at

mmb.irbbarcelona.org/molywood

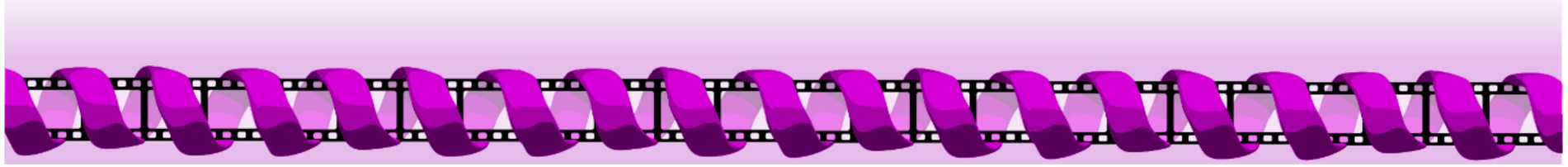
(& looking forward to questions)

Bioinformatics, 2020, 1–2
doi: 10.1093/bioinformatics/btaa584
Advance Access Publication Date: 23 June 2020
Applications Note

Structural bioinformatics

Molywood: streamlining the design and rendering of molecular movies

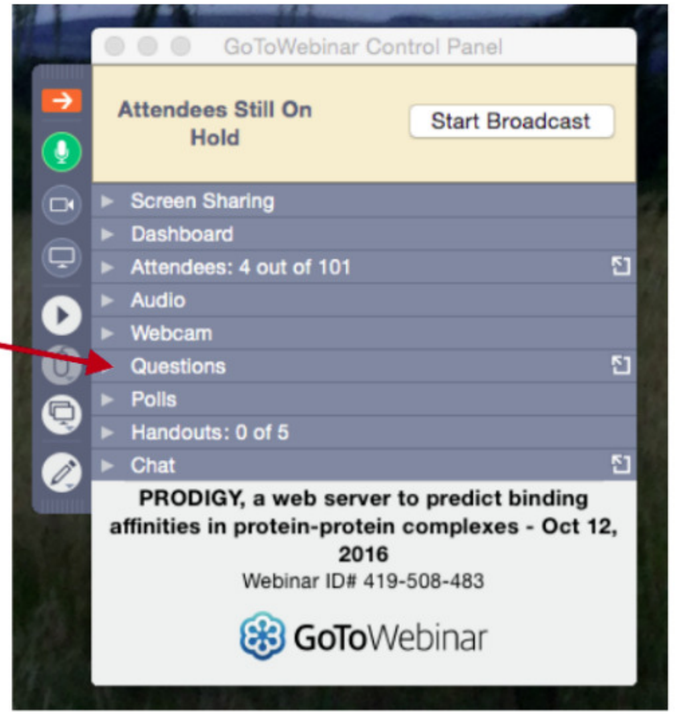
Miłosz Wieczór[1,2,*], Adam Hospital[2], Genis Bayarri[2], Jacek Czub[1] and Modesto Orozco[2,3,*]



Audience Q&A session

- Please use the Questions function in GoToWebinar application
  - If you *don't have audio*, please mention that in the question.

- Any other questions or points to discuss after the live webinar? Join the discussions at http://ask.bioexcel.eu.



Next autumn BioExcel webinar

5 November at 15:00 CET

Using competencies to guide training and professional development

by *Vera Master and Marta Lloret Llinares*

See https://bioexcel.eu/