

KLT picker, a user guide

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December, 2019

1 Downloading the KLT picker

The current version of the KLT picker is available for users with MATLAB. In the near future we plan to release a Python version. Download and extract the package from

`https://`

The extracted directory has the following structure

- `KLTpicker_start` Main script.
- `userManual` The documentation for the package.
- `LICENSE` The package license.
- `README` A short README file for the package.
- `matlab/` The MATLAB source code. This contains all the functions needed to run the KLT picker.
- `get10028` Script to download micrographs for the Example Section 3.
- `example/` This directory will be used in Section 3 to demonstrate the use of the KLT picker on a real dataset from the EMPIAR repository [1].

2 Running the KLT picker

After downloading the package, start MATLAB in the package directory and run

`KLTpicker_start`

The following question will appear, one by one, on the Command Window

Enter full path of micrographs MRC file:

Type the path to the directory which contains the micrographs MRC file.

Enter full path of output directory:

Type the path where the particles coordinate files will be saved.

Enter the particle size in pixels:

Type the particle diameter size in pixels.

pick all particles?(Y/N)? [Y]

Type Y to pick all possible particles. If you type N then the following question will appear

How many particles to pick:

Type the number of particles to pick per micrographs.

Pick noise images?(Y/N)? [N]

Type N if you don't want to pick noise images. If you type Y then the following question will appear

How many noise images to pick:

Type the number of noise images to pick per micrographs.

Do you want to use the GPU?(Y/N)? [Y]

Type Y to use the GPU and N to not use it.

The KLT picker will start and will display progress notifications. The outputs are the coordinate files (box and star) and a text file that summarize the picking process at the output directory.

3 Example

In this section we will demonstrate the use of the KLT picker on 5 micrographs of EMPIAR-10028 (Plasmodium Falciparum 80S ribosome) [2] from the EMPIAR repository [1].

Start MATLAB in the package directory and run the following

```
get10028 # downloading 5 micrographs to ./example/micrographs
directory.
```

```
KLTPicker_start
```

```
Enter full path of micrographs MRC file:
./example/micrographs/
```

```
Enter full path of output directory: ./example/results
```

```
Output directory does not exist. Create?(Y/N)? [Y] Y
```

```
Enter the particle size in pixels: 300
```

```
pick all particles?(Y/N)? [Y] Y
```

```
Pick noise images?(Y/N)? [N] N
```

```
Do you want to use the GPU?(Y/N)? [Y] Y
```

When finished, the KLT picker will display the message: **Finished the picking successfully.** In order to display the picking results in EMAN [3], open the terminal in the package directory and create a new directory named **eman**. Change directory to **eman** and enter the following code one by one.

```
e2rawdata.py ../example/micrographs/*.mrc --invert --edgenorm
--xraypixel --ctfest --apix=1.0 --voltage=200.0 --cs=2.0
--ac=10.0 --threads=4 --defocusmin=0.6 --defocusmax=4.0
```

```
e2import.py
../example/results/pickedParticlesParticleSize300/box/*.box
--import_boxes --box_type=boxes
```

```
e2boxer.py --allmicrographs --boxsize=300 --ptclsize=300
--apix=1.0 --no_ctf --gui --threads=4
```

In order to display the picking results of the **first** micrograph in RELION [4], open the terminal in the package directory and create a new directory named **relion**. Change directory to **relion** and enter the following code.

```
relion_display --i ./example/micrographs/001.mrc --coords
./example/results/pickedParticlesParticleSize300/star/001.star
--scale 0.15 --particle_radius 150 --angpix 1 --lowpass 20
--pick
```

In order to display the picking results of the n'th micrograph change **001.mrc** and **001.star** in the code above to **00n.mrc** and **00n.star**.

3.1 Citation

If you use the KLT picker, please cite our paper “KLT picker: Particle picking using data-driven optimal templates”, available at <https://>.

References

- [1] Iudin, A., Korir, P., Salavert-Torres, J., Kleywegt, G., and Patwardhan, A. (2016). *EMPIAR: A public archive for raw electron microscopy image data*. Nature Methods, 13.
- [2] Wong, Wilson and Bai, Xiao-chen and Brown, Alan and Fernandez, Israel S and Hanssen, Eric and Condrón, Melanie and Tan, Yan Hong and Baum, Jake and Scheres, Sjors H W. (2014). *Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine*. Wong et al. eLife ,3,e03080.
- [3] G. Tang, L. Peng, P.R. Baldwin, D.S. Mann, W. Jiang, I. Rees & S.J. Ludtke. (2007). *EMAN2: an extensible image processing suite for electron microscopy*. Journal of structural biology, 157, 38-46.
- [4] Scheres, Sjors HW. (2015). *Semi-automated selection of cryo-EM particles in RELION 1.3*. Journal of structural biology, 128, 114-122.