The Help File of *KinomeX*

(Version 1.20)

Contents

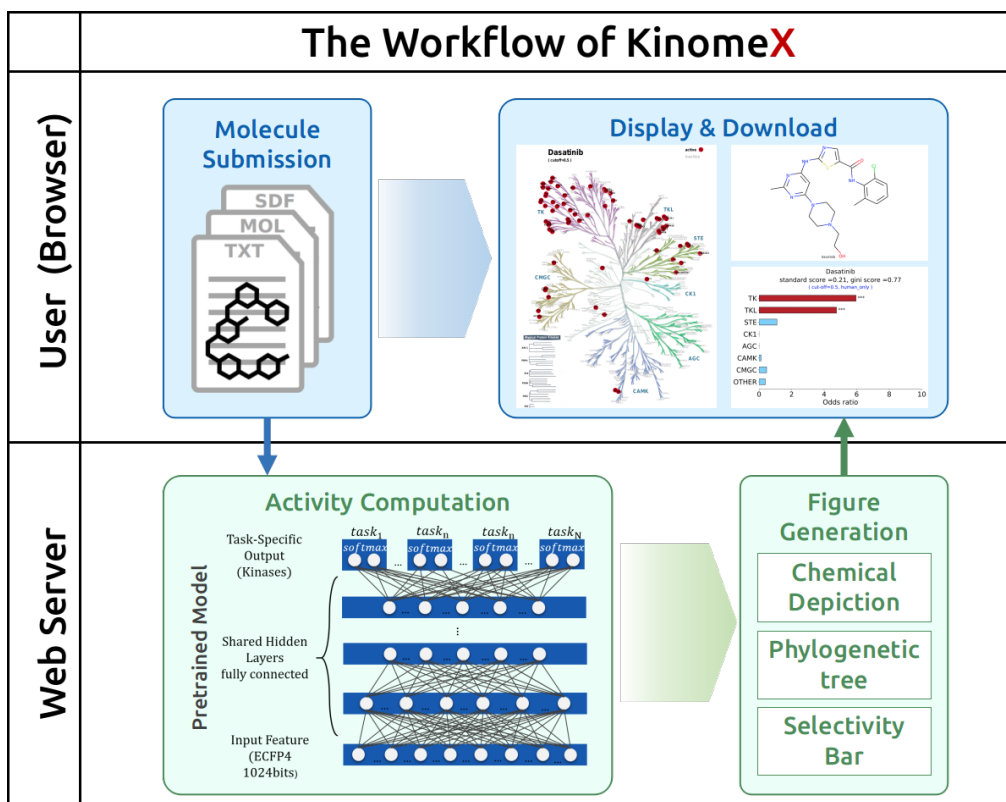## i.   Overview of *KinomeX*

Fig. 1 The workflow of KinomeX

ii.   How to use *KinomeX* for kinome prediction

A typical kinome-wide virtual profiling workflow of *KinomeX* is as following:

1) A molecule is submitted from user-side(browser) by drawing or by uploading a mol/sdf/txt file (Molecule Submission);

2) The kinome-wide activities are computed by server-side based on a pretrained Multi-task Deep Neural Network(MTDNN) model (Activity Computation);

3) Figures with three cut-offs of activities are generated based on the profiling, including a chemical depiction, a kinase phylogenetic tree and a selectivity bar (Figure Generation);

4) Results download and/or display online.

For the steps from 1 to 4, user actions using web browser are required. Here we present the operation methods for these steps.

Step 1

Two types are supported for inputting a molecule: <DRAW> and <UPLOAD>.   As long as the input molecule is valid, it can then be put into a submission list for further processing. A maximum of **5 molecules** can be added to the submission list.
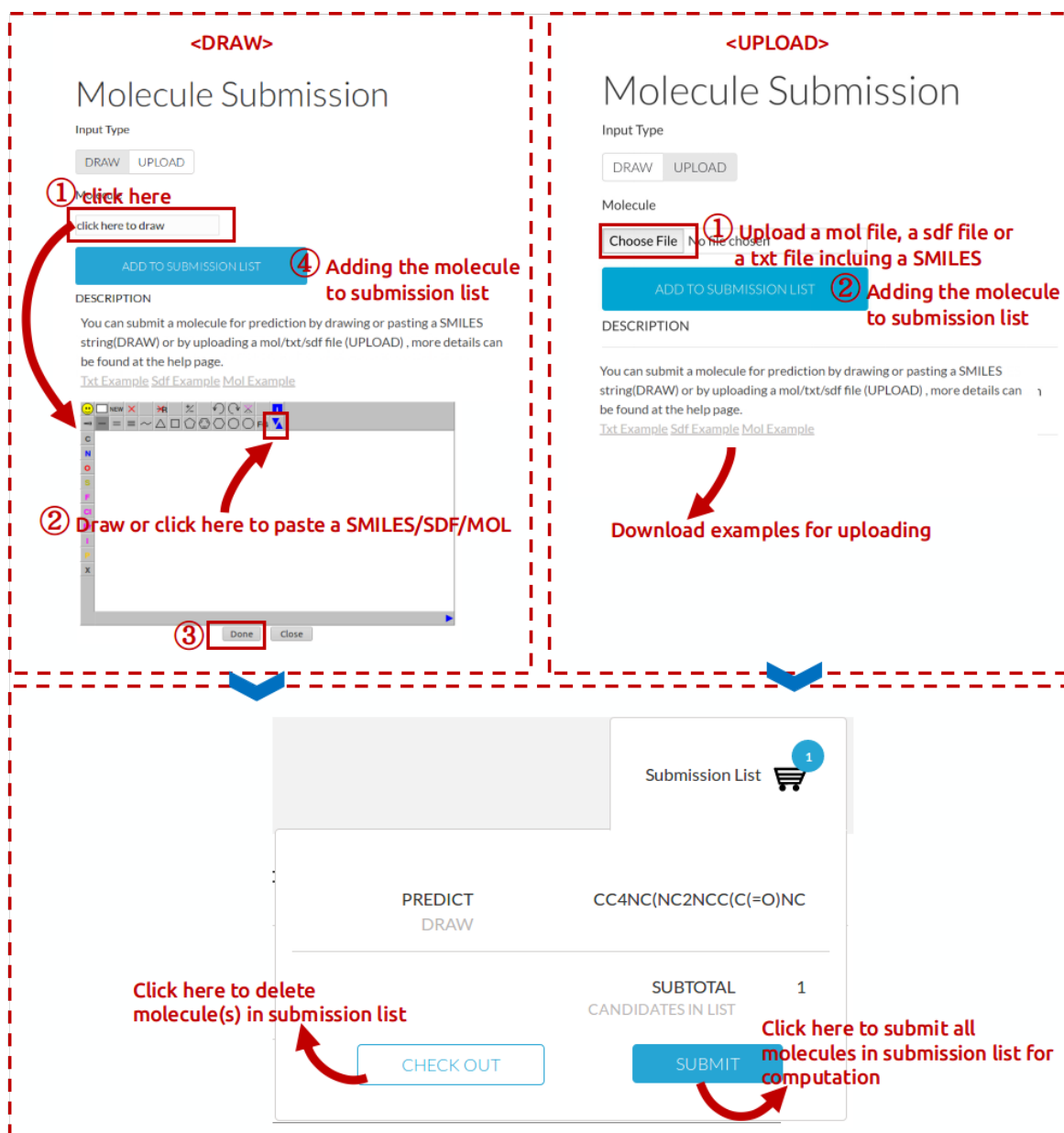
Fig. 2 Step I of *KinomeX* workflow

Steps 2-4

Once the molecules in list are submitted, the job record page will show up and automatically refreshed in every 10 seconds. The calculation period for a molecule will take about 60 seconds, which covers both the activity computation and the figure generation steps. In the end, two "zip" files including all the figures and details of these calculations can be downloaded, and the figures can also be viewed online.

SUBMIT   HELP   ABOUT

Home / Record / 16bf803f-7113-4ff1-9e16-0d1756c515f6 (Automatically refresh, ETC 60 seconds per job after starting to run.)

Click here to see the figures online

MOLECULES	COMPUTING STATUS	COMPUTING RESULTS	PRESENTING STATUS	PRESENTING RESULTS
Cc4nc(Nc2ncc(C(=O)Nc	done	⬇	done	Ready to show ⬇

**Click here to download
a "zip" file including:**

**Click here to download
a "zip" file including:**

⚙ 20181229175235.svg **Chemical depiction**

📄 data.txt **SMILES and name(or an
automatically generated id)**

📄 mapping.csv **Information of predicted kinases**

📄 prediction_all.csv **Probabilities whether the molecule is active
active against human/rat/mouse/... kinases**

📄 prediction_human.csv **Probabilities whether the molecule is
active against human kinases**

- ▼ 📁 all **human/rat/mouse/... kinases**
  - ▼ 📁 c_0_5 **Cut-off = 0.5**
    - 📄 phylogenetictree_fig **Figure of phylogenetic tree**
    - 📄 selectivity_fig **Figure of selectivity bar**
    - 📄 selectivity.csv **Detail of selectivity**
  - ▶ 📁 c_0_7
  - ▶ 📁 c_0_9
- ▼ 📁 human **human kinases**
  - ▶ 📁 c_0_5
  - ▶ 📁 c_0_7
  - ▶ 📁 c_0_9

Home / Record / d080f088-da32-44fb-9ff1-541eeb6f615a / Figure (Cutoff: 0.5) **cutoff (= 0.5 here)**   ALL HUMAN ONLY

**The location of the profiled kinases and predicted active
interactions is shown in a kinase phylogenetic tree**

Chemical depiction

20181229185954
(cutoff=0.5)

Legend:
● active
  inactive

**Molecule name(or an
automatically generated id)**

**Predicted as
acitve when the
cutoff is set to
0.5**

**Predicted as
inacitve when
the cutoff is set
to 0.5**

TK   TKL   STE   CK1   CMGC   AGC   CAMK

Kinome Profiling

ALL / HUMAN ONLY

20181229185954OH

Chemical Structure

**Overall   selectivity for
[human only]/ [all] kinases**

Selectivity

20181229185954
(cutoff=0.5, human_only)
standard score =0.21, gini score =0.77

TK   ***
TKL   ***
STE
CK1
AGC
CAMK
CMGC
OTHER
      0   2   4   6   8   10
         Odds ratio

**Sub-group selectivities
for [human only]/ [all] kinases**

Selectivity

« | 1 | 2 | 3 | »   **Click here to select 3 cutoffs (0.5, 0.7, 0.9)**

Fig. 3 Steps 2-4 of *KinomeX* workflow

iii.   Submission List，Job and Record

Submission list, job and record are the terms in *KinomeX* for data processing. Details of which are explained as follows:

A. Submission List

A submission list is a temporary location for jobs to be executed, with each of the job having valid inputs for the next steps in the workflow. People can delete any improper submissions as needed, and submit them to the server for processing.

B. Job

A job refers to a standard data processing unit in *KinomeX*, which should possess valid inputs (molecules) and outputs (computing results and figures), as well as the typical 4 steps of *KinomeX* in its life cycle. According to different situations, a job may be at various statuses such as "queue", "running", "done", "error", etc. A job with a "done" sign at computing status means the process of activity computation is finished, and a "done" sign at presenting status denotes to the termination of figure generation.

C. Record

A record consists of several jobs submitted at the same time, within a same submission list. As for

convenience, users can submit as many as **5 jobs (molecules)** simultaneously.

iv.   Miscellaneous

A. Max number of jobs

There is no upper limit to the number of jobs. However, only up to **5 jobs (molecules)** can be submitted simultaneously, in other words, five jobs per record at the top.

B. Time consumption of a job

Basically, a job's computing process (including activity computation and figure generation) takes about 60 seconds. Due to the limitation of computing resources, jobs submitted from all of the users may be forced into a waiting list before run. So a little patience may be needed while a lot of jobs waiting for processing.

C. Browser compatibility

KinomeX uses a few techniques for data processing and visualization conveniently, yet the web browsers without supporting modules cannot be functioning properly. A few supported web browsers are listed in Table. 1.

Table 1. Supported web browsers of *KinomeX*

Browser	Version
Chrome(Windows, Linux)	71.0.3578.98
Opera(Windows)	56.0.3051.116
Firefox(Windows, Linux)	63.0.3

D. Data storage time

On *KinomeX*, a maximum of **7 days** of the job records will be stored, so we strongly recommend users to **download all of the results and figures** at their suitable times. Besides, one can clear all of their job records as long as it is needed. The server will keep neither the computation results nor the related database entries, as to guarantee the safety of the users' private data.