The manual for FFI-Net V1.0

1. Introduction

A deep learning program, called fast fluorescent identification network (FFI-Net), is designed to fast identify the fluorescent components in the single three-dimensional excitation-emission matrix (3D-EEM) spectrum. All deep learning models were pretrained and the weights of pretrained deep learning model were saved as '.h5' file.

2. Requirements

(1) Create Anaconda environment with python 3.7 in Anaconda prompt:

```
conda create -n py3.7 python=3.7
```

(2) Activate the py3.7 environment:

```
conda activate py3.7
```

(3) Install other requirements (Table 1):

Table 1 The version and installation of requirements

Requirements	Version	Installation
tensorflow	2.2.0	pip install tensorflow==2.2.0
keras	2.3.1	pip install keras==2.3.1
matplotlib	3.3.4	pip install matplotlib
pandas	1.2.3	pip install pandas
openpyxl	3.0.7	pip install openpyxl
scikit-learn	0.24.1	pip install scikit-learn
PyQt5	5.15.4	pip install pyqt5
PyQt5-tools	5.15.2	pip install PyQt5-tools

(4) Set environmental variable of PyQt5-tools and environmental path of PyQt5

3. The application of the FFI-Net V1.0

3.1 Prepare data

The setting of the 3D-EEM fluorescence spectroscopy (Ex/Em range and interval) should fulfill the requirements of our approach (Ex>200-450 nm, Ex have 200+5n nm, Em>250-500 nm and Em have 250+5n nm). The data of 3D-EEM spectrum recorded by the 3D-EEM fluorescence spectroscopy should be saved in Excel file ('.xls' or '.xlsx'). The Raman scatter in the 3D-EEM spectrum should be removed by subtracting the pure water spectrum from the sample spectrum. The example of the Excel file can be found in the Test data for FFI-Net folder.

3.2 Open user interface

(1) Completely download https://github.com/RunzeXu1314/FFI-Net.git;

(2) Unzip all '.rar' files in the Weights folder to achieve the weights of pretrained deep learning models. Put all weights.h5 files in the Weights folder;

(3) Open the Anaconda Prompt;

(4) Enter the location where you download the FFI-Net files:

```
cd C:\Users\RunzeXu\UI (change this location)
```

(5) Activate the py3.7 environment:

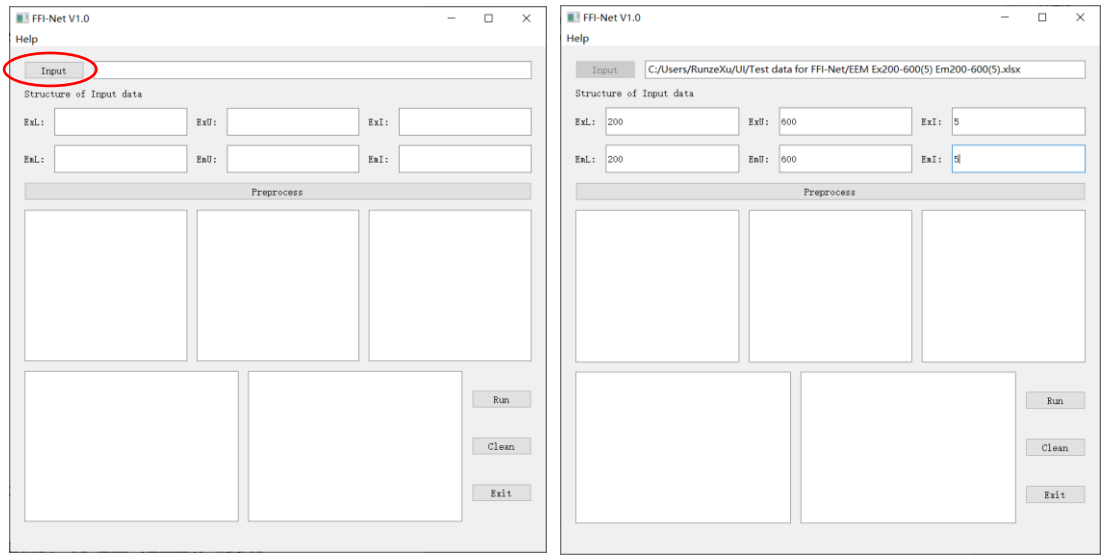
```
conda activate py3.7
```

(6) Open the user interface:

```
python main.py
```

3.3 Input data

Click the ‘Input’ button, and select your Excel file that saves the 3D-EEM spectrum. Input the example in the Test data for FFI-Net folder to test the FFI-Net.



Entering the structure of the input data including lower boundary of Ex (ExL), upper boundary of Ex (ExU), Ex interval (ExI), lower boundary of Em (EmL), upper boundary of Em (EmU) and Em interval (EmI).

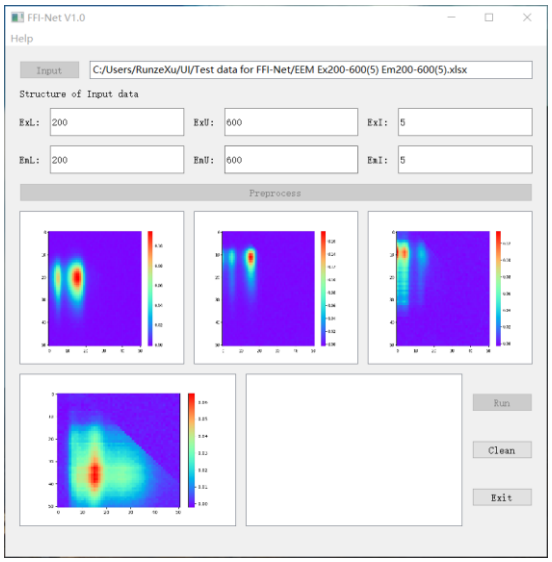
3.4 Preprocess data

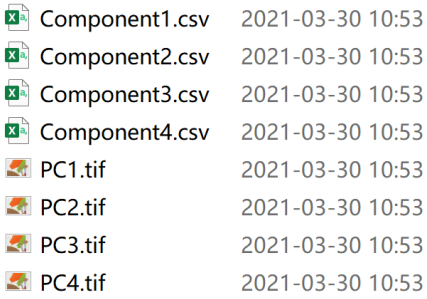
Click the ‘Preprocess’ button to preprocess the input data to a unified format. The preprocessed data will be generated in the Preprocess folder.

column data.csv	2021-03-30 10:39	Microsoft Excel ...	30 KB
row data.csv	2021-03-30 10:39	Microsoft Excel ...	19 KB

3.5 Simulate data

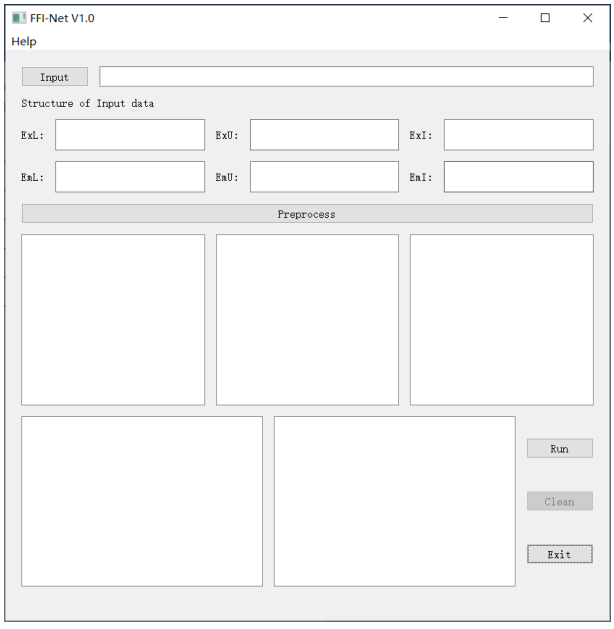
Click the ‘Run’ button to start the deep learning simulation process. The simulation results will present on the user interface, and the data of fluorescent components will be saved in the Results folder. User need to save these results by copying them to other folder before doing another simulation.





3.6 Clean data

User need to save their results by copying the files in the Results folder to other folder before using this function. Click the 'Clean' button to remove the files generated in the Preprocess and Results folders, and release the 'Input' and 'Preprocess' button. Then, user can start another simulation by repeating **3.3-3.6**.



3.7 Close the interface

Click the 'Exit' button to close the interface and remove the files generated in the Preprocess and Results folders at the same time.

4. Limitations

We demonstrate that the accuracy of the FFI-Net will be further improved when more 3D-EEM data is available as a train dataset. Therefore, we sincerely hope that researchers with qualified 3D-EEM data can send their data to the email (runzexu@hhu.edu.cn) to help us enlarge the training dataset. We will continuously update the version of the FFI-Net and express our gratitude in the help section of the FFI-Net to researchers who provide their data.