GPS Manual

Group-based Prediction System

Version 6.0 22/4/2023

Author: Miaomiao Chen, Weizhi zhang and Yu Xue*

Contact: Miaomiao Chen, chenmiaomiao@hust.edu.cn, Weizhi zhang, zhangweizhi@hust.edu.cn, Yu Xue, xueyu@hust.edu.cn The software is only free for academic research. The latest version of GPS software is available from https://gps.biocuckoo.cn/download.php. Copyright (c) 2004-2023. The CUCKOO Workgroup. All right reserved.

Statement

1. **Implementation**. The softwares of GPS 6.0 are implemented in Python. Usually, both of online service and local stand-alone packages will be provided.

2. **Availability**. Our softwares are freely available for academic researches. For nonprofit users, you can copy, distribute and use the softwares for your scientific studies. Our softwares are not free for commercial usage.

3. **GPS**. Previously, we used the GPS to denote our Group-based Phosphorylation Scoring algorithm. Currently, we are developing an integrated computational platform for post-translational modifications (PTMs) of proteins. We re-denote the GPS as Group-based Prediction Systems. This software is an indispensable part of GPS.

4. **Usage**. Our softwares are designed in an easy-to-use manner. Also, we invite you to read the manual before using the softwares.

5. **Updation**. Our softwares will be updated routinely based on users' suggestions and advices. Thus, your feedback is greatly important for our future updation. Please do not hesitate to contact with us if you have any concerns.

6. **Citation**. Usually, the latest published articles will be shown on the software websites. We wish you could cite the article if the software has been helpful for your work.

Download & Run

The software of GPS 6.0 was implemented in Python, and could run on Windows, mac OS and Linux systems. The distributions can be found at <u>https://gps.biocuckoo.cn/download.php</u>.

Both of the software and the pre.zip file need to be downloaded for full functionality. After downloading, please unzip the pre.zip file to the directory where the software is located.

pre	2023/4/20 21:23
GPS_6.0_windows	2023/4/21 0:21
🔂 pre	2023/4/21 19:27

Then, please double-click on the file GPS_6.0_windows.exe to begin run it. It may take some time (especially on mac OS), please wait patiently. And snapshot of the program is shown below:

📧 GPS 6.0						- 🗆	×
File Tools Help							
PKs	Predicted sites						
 Phosphorylation Serine/threonine kinase AGC CAMK CK1 CMGC PKL RGC STE TKL Atypical Other Tyrosine kinase TK 	Position	Code	Kinase	Peptide	Score	Cutoff	~
	Threshold			Console			_
	🔿 High 🛛 🖲) Medium 🔿 L	w O All	Example	Clear	Submit	

Q & A

Windows

Q: The software could open, but run fails after clicking the "Submit" button. What to do to solve this problem?

A: First, please check if the pre.zip file is unpacked and locates in the same folder where the .exe software is located.

If it is right, then follow steps below to run the software:

First, open the terminal on your computer.

Second, go to the path where the software and "pre" file folder are placed.



Third, drag the software to the terminal, and then click the Enter key.



Finally, it will work for prediction of the kinase-specific phosphorylation sites.

E GPS 6.0						- 🗆 🗙	
File Tools Help							
PKs	Predicted sites						
Phosphorylation A Soring (throoping kings)	Position	Code	Kinase	Peptide	Score	Cutoff	
Serine/threonine kinase	>ESR1						
> _ CAMK	104	s	Atypical/PIKK	FPPLNSVSPS	0.0301	0.0185	
> CK1	106	s	Atypical/PIKK	PLNSVSPSPL	0.0540	0.0185	
> CMGC > PKL	118	s	Atypical/PIKK	LHPPPQLSPF	0.0471	0.0185	
> 🗌 RGC	154	s	Atypical/PIKK	PAFYRPNSD	0.0189	0.0185	
	294	s	Atypical/PIKK	RAANLWPSP	0.0484	0.0185	
 > BCR > GTF2F1 > POHK ~ PIKK > ATM > ATR > DNAPK ~ FRAP > MTOR TOR2 > SMG1 _ PIKSCA _ RIO 	Enter requence(s) in FASTA format >ZSSN MITHITIAGGMALLINIQORELEFINERGLATIERFLGEVILOSSN AVTHYEGAATEFMAAAANAGVOQTOLFVOROSEAAAFOSNELOOFFFLM SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOODALMANSONELMANGADAAAAAA SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOODALMANSONELMANGADAAAAATAGVOQTOLFVOROSEAAAFOSNELOOFFFLM SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOODALMANSONELMANGADAAAAAAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOODALMANSONELMANGADAAAAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOODALMANSONELMANGADAAAAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOOTALMANSONELMANGADAAAAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOOTALMANAAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOOTALMANAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOOTALMANAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENE ATAGKITUMENGAANAAFTATERMINOOTALMANAATAGVOQTOLFVOROSE SSSSFJULIOSSNONENAAAAATAGVOTTILIDAAAATAGVOQTOLFVOROSEAAATAGVOQTON SSSSFJULIOSSNONENAAAAAATAGVOTTILIDAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAAATAGVOQTOLFVOROSEAAAAAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAATAGVOQTOLFVOROSEAAATAGVOQTOLFVOROSEAATAGVOQTOLFVOROS						
> Other	Threshold			Console			
✓ ✓ Tyrosine kinase → □ TK ✓	⊖ High (● Medium 🔿 I	.ow () All	Example	Clear	Submit	

Mac OS

Q: What to do when the downloaded GPS6 file is a document file, not an exec file?

A: Open the Terminal on mac, then input "chmod -x /path/GPS6" and click the enter button to change the document to EXEC file.

```
(base) tiaotiaoma@tiaotiaomadeMacBook-Air ~ % chmod +x /Users/tiaotiaoma/Desktop/cmm/test_web/GPS6
(base) tiaotiaoma@tiaotiaomadeMacBook-Air ~ %
```



GPS6

Q: I was trying to install the software on mac but my installer says the file is unsafe. How can I properly install the software in Mac OS?

A: By default, Mac OS only allows users to run applications from 'verified sources'. In effect, this means that users are unable to run most applications downloaded from the internet. You can follow the directions below to prevent this error message from appearing.

(1) Open the Preferences. This can be done by either clicking on the System Preferences icon in the Dock or by going to Apple Menu > System Preferences.

(2) Open the Security & Privacy pane by clicking Security & Privacy.

(3) Make sure that the General section of the Security & Privacy pane is selected. Click the icon labeled Click the lock to prevent further changes.

(4) Enter your username and password into the prompt that appears and click Unlock.

(5) Under the section labeled Allow applications downloaded from, select Anywhere. On the prompt that appears, click Allow From Anywhere.

(6) Exit System Preferences by clicking the red button in the upper left of the window. You should now be able to install and run applications downloaded from the internet.

Linux

Q: I can't run the downloaded GPS6 software downloaded from web in Linux. How can I open and run it?

A: Open the Terminal on the computer, then input "chmod -x /path/GPS6" and click the enter button. Then you could run this software smoothly.

e Tools Help	_	GPS 6.0	_	_	_	e	0
3	Predicted sites						
 Serine/threonine kinase AGC CAMK CK1 CMGC PKL RGC STE TKL Atypical Other Tyrosine kinase TK 	Position	Code	Kinase	Peptide	Score	Cutoff	
	Threshold			Console			