## WEBSERVER FOR DEEPKINZERO

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#### ABSTRACT

#### DeepKinZero

Zero-Shot Learning for Predicting Kinase-Phosphosite Associations Involving Understudied Kinases



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#### Latest Updates

New Updates For DeepKinZero:

Update date: ##,##,####

2019 sees the redesign of our website. Take a look around and let us know what you think. Welcome to DeepKinZero: The Newest Approach for Predicting Kinases

DeepKinZero is specifically designed for making predictions for under-studied Kinases with no known phosphorylation sites. By analysis and training through data sets of known kinases, the model is capable of establishing a pattern for determining binding affinity and compatibility between kinases and protein sequences.

### **PROJECT DETAILS**

| DeepKinZ<br>Zero-Shot Learning for Pred | ero<br>licting Kinase-Phosphosit | te Associations Invo | lving Underst | udied Kinases | <b>O</b>    |
|---|----------------------------------|----------------------|---------------|---------------|-------------|
|   |                                  | Home Submit          | Tutoria       | l About       | Contact Us  |
|   |                                  |                      |               |               |             |
| Latest Updates                          |                                  |                      |               |               |             |
| New Updates For<br>DeepKinZero:         |                                  |                      |               |               |             |
| Update date: ##,##,####                 | UniProt ID                       | Protein              | Sites         | Kinase        | Probability |
| 2019 sees the redesign of               |                                  | i i oteni            | Sites         | Amase         | riosasinty  |



Phosphorylation is a post translational modifications which is the key regulatory mechanism of intercellular signaling networks by changing the activity and structure of the protein through addition of a phosphate group to amino acid residues. The enzyme responsible for such key mechanism is called a "kinase". Almost every protein can be phosphorylated from varying sites (Dupré, 2017). Also, there are over 600 different kinases for Homo sapiens. So, detecting which kinase is responsible for the phosphorylation of which site remains a question.

DeepKinZero is a ground breaking method for making such predictions for kinases with no known sites. The concept of using known sites and kinase pairs to establish a pattern that can be used for predicting the affinity of any kinase for a given site creates a new field for studying under-studied kinases which makes this method so significant.

The aim of this research is designing a webserver so that the findings of DeepKinZero and the potential it holds can be used for any scientist. It is known that the hyperactivity, malfunction or overexpression of any gene can be triggered by phosphorylation and is very much linked with series diseases like cancer (Ardito, 2017). So, creating accessibility for such a tool is a great value for the hope of treatment for such diseases.

| around and let us know what you think.  | <u>Q00653</u> | NFKB2_HUMAN | 707 | GSK3B   | 1.0   |
|---|---------------|-------------|-----|---------|-------|
| Read more   | <u>Q00653</u> | NFKB2_HUMAN | 715 | CSNK2A1 | 0.984 |
|   | <u>Q00653</u> | NFKB2_HUMAN | 713 | CSNK2A1 | 0.984 |
| Similar Prediction<br>Tools   | <u>Q00653</u> | NFKB2_HUMAN | 416 | CSNK2A1 | 0.984 |
| <ul> <li><u>Musite</u></li> <li><u>Predikin</u></li> </ul>  | <u>Q00653</u> | NFKB2_HUMAN | 658 | CSNK1G2 | 0.926 |
| <ul> <li><u>PhosphoPick</u></li> <li><u>KinomeXplorer</u></li> <li><u>Kinexus PhosphoNet</u></li> </ul> |               |             |     |         |       |

The most important app which is the Submission page hosts the input view as well as the outputted results. The input screen enables user to enter the substrate of interest by its UniProt ID along with the amino acid position to be phosphorylated. By such small information the model can predict the kinase with high accuracy.

As output, a table containing the predicted kinase with a probability score that reflects the liability of the predicted kinase having high binding affinity to be actually responsible for that phosphorylation event is displayed. In the displayed table the following data is available:

#### UniProt ID that was inputted

- Proteins code in NCBI database
- Site that was inputted
- Kinase that is predicted by DeepKinZero

#### **OBJECTIVE**

Development of a webserver that will serve as an interface for the newly developed machine learning model DeepKinZero.

The model makes predictions for matching under studied kinases with their complementary substrate phosphorylation sites by training through datasets of known kinase-phosphorylation site pairs.

The webserver simplifies a complicated algorithm into a website so that the benefits of DeepKinzero can cater to any scientist.



#### Site Score for that particular kinase

#### CONCLUSION

As the outcome of our work, a new tool that is capable of making meaningful predictions even for unknown kinases is ready to be presented to the community of science. The neat design as well as the detailed tutorial part which demonstrates a sample input and output that clarifies the interpretation of results is aimed to be user friendly and understandable by any scientist. By serving as a tool, the aim of catering the complicated machine learning algorithm of DeepKinZero to scientists is accomplished.

By the information that is predicted from DeepKinZero tool, many facilities and researches can access the data provided by DeepKinZero to study underexplored kinases that might be related for treatment of diseases by targeted therapy approaches and nano-drug development.

A platform that carries all the necessary apps such as Submission page, details on the article, contacts, databases and so on was created for a userfriendly interface that is sophisticated and easily understood.

| r Prediction   | 707, 715                      |   |
|--|-------------------------------|---|
| <u>te</u><br><u>phoPick</u><br><u>meXplorer</u><br><u>xus PhosphoNet</u> | Upload File<br>Output Options | Dosya Seç Dosya seçilmedi<br>Display The Predicted Kinase |

Since the coding language of DeepKinzero is Python, the framework that was used to establish an interface design that the main code runs under was chosen to be Django as it facilitates the code as well as supplying a base for web development.

#### REFERENCES

Ardito, F., Giuliani, M., Perrone, D., Troiano, G., & Lo Muzio, L. (2017). The crucial role of protein phosphorylation in cell signaling and its use as targeted "rapy (Review). *International journal of molecular medicine*, *40*(2), 271–280. doi:10.3892/ijmm.2017.3036

Dupré, A., Jessus, C. (2017). Protein Phosphorylation. *Centre national de la recherche scientifique*, 10.5772/intechopen.71332. pub109.3085915