

# InCharge- Operation Manual



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## What is InCharge?

InCharge is a program allowing you to predict a **pl point** and **charge** of a protein/peptide at various pH levels. In comparison to its analogues, InCharge provides a more precise result (tested in a large selection of human, bacterial and other molecules with a known pl point, which was determined by physical methods).

## Entering the Data

To analyse the sequence, simply **Paste** it into the **Sequence** window . We recommend also entering the accession number of the sequence you use and the name of your sequence or project. This data will be present in all **Results** you save after the analysis.

The screenshot shows the InCharge web interface. It has three main input sections: 'Protein Name', 'Accession Number', and 'Sequence in FASTA'. The 'Protein Name' and 'Accession Number' fields are empty text boxes. Below the 'Accession Number' field is a 'Clear' button and a dropdown menu with the text '---Select a demo sequence---'. The 'Sequence in FASTA' field is a large text area containing the text 'Enter the amino acid sequence in 1-letter code (FASTA)'. A blue box highlights a 'Filter' checkbox which is checked. Below the text area is another 'Filter' checkbox (unchecked) and two input boxes for 'Start:' and 'End:', both containing the number '0'.

If your sequence contains gaps (may appear due to formatting) or contains abnormal signs (punctuation/letters that are not amino acid code) the analysis will be aborted. To avoid it, keep the “Filter” option selected.

To analyse only a fragment of the sequence, please enter the position number of the first and the last amino acids of the fragment you want to analyse. Please be aware that the numeration of the sequence starts from the first amino acid of the original sequence and will be kept during the analysis of the fragment. For example, if the first aa of the fragment was 101 it will be indicated as 101 in all further analysis and Results.

However, if you paste a sequence fragment into the **Sequence** window, its first amino acid will be referred to as position 1, not the position in the original sequence - source of the fragment.

## Demo sequences

For your training purposes we provide several sequences with different pl point to test the program. You may choose them by selecting from the drop-down **-Select a demo sequence-** list.

The pl point defined for these molecules by physical methods is provided on the title of a sequence.

Clear

MAEKRNIFLV  
DREEKVINEL  
PLLHVETPPR

---Select a demo sequence---

- pl=5.29 - Shikimate kinase 1 [E.coli]; P0A6D7
- pl=5.03 - Deoxyuridine 5'-triphosphate nucleotidohydrolase [E.coli]; P06968.2
- pl=4.68 - Protein GrpE (=HSP24; HSP-70 cofactor) [E.coli]; P09372.1
- pl=7.06 - PPIase/FKBA (mature chain: positions 26-70) [E.coli]; P45523.1
- pl=5.12 - DNA-directed RNA polymerase subunit beta [E.coli]; P0A8V2.1

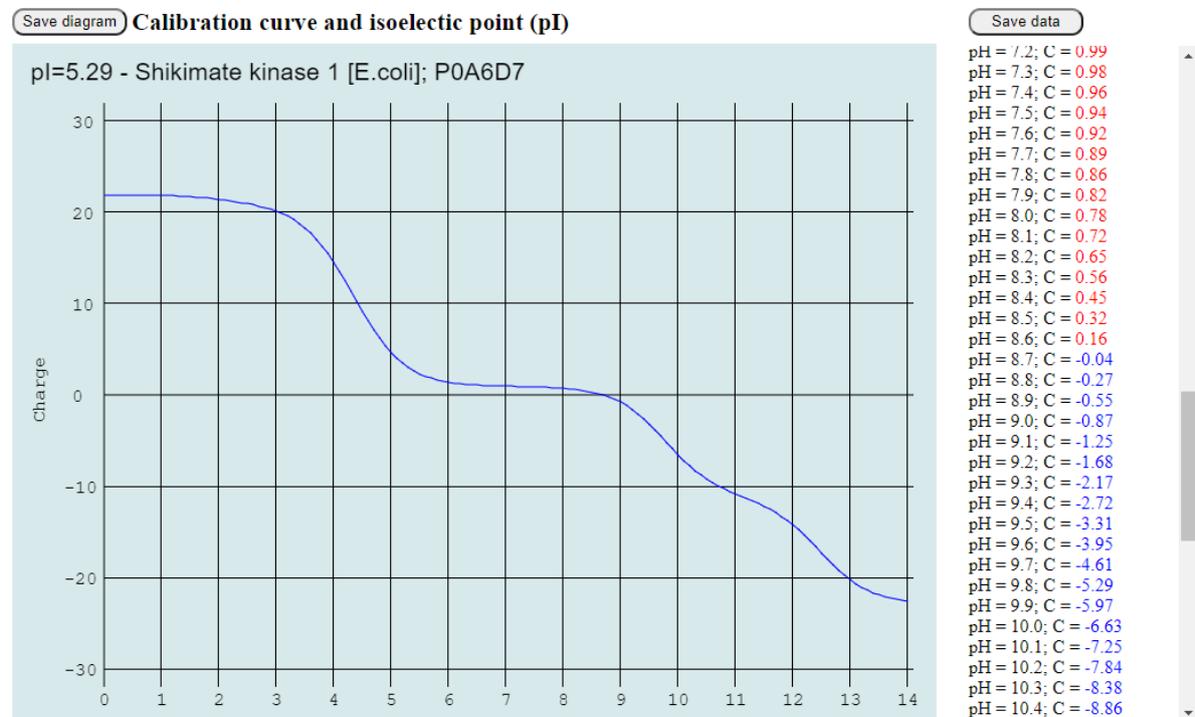
Filter

## Viewing and saving the Results

The results of the analysis are provided as calibration curve graphic as well as a table with pH steps of 0.1

## Whole Molecule Profile

Protein name: pI=5.29 - Shikimate kinase 1 [E.coli]  
Sequence length: 173aa  
Fragment: 1 - 120



You may **Save** the diagram (*Save diagram* button) as a 96 ppi *PNG* file. To have a name of the protein shown in the image do not forget to fill the Protein Name section in data entry section.

You may **Save** the tabular report (*Save data* button) for your records as a standalone *HTML* document that may be further converted into other formats.