

**Title of Manuscript:** Peptide Combination Generator: A tool for generating peptide combinations.

**Authors:** Naseem Ali, Arzoo Shamoan, Neelesh Yadav\*, Tanuj Sharma\*

**Affiliation:** Bioinformatics Center, Forest Research Institute, Dehradun, Uttarakhand, 248006, India.

**Supplementary Data:**

**Table s1:** The table summarizes the twenty amino acids differentiated into six broad group, along with three letter and single letter code.

Sr. No.	Nature	Name of Residue	Three Letter Code	Single Letter Code
1	Acidic	Aspartic Acid Glutamic Acid	Asp Glu	D E
2.	Basic	Arginine Histidine Lysine	Arg His Lys	R H K
3.	Hydrophobic (Aliphatic)	Alanine Isoleucine Leucine Methionine Valine	Ala Ile Leu Met Val	A I L M V
4.	Aromatic	Phenylalanine Tryptophan Tyrosine	Phe Trp Tyr	F W Y
5.	Polar (Uncharged)	Asparagine Cysteine Glutamine Serine Threonine	Asn Cys Gln Ser Thr	N C Q S T
6.	Unique	Glycine Proline	Gly Pro	G P

## Images:

The image shows the main web server front page for the Peptide Combination Generator. At the top, there is a navigation bar with links for 'About', 'Feedback', and 'Contact Us'. The main heading is 'Peptide Combination Generator' with a subtext: 'A tool for generating all the possible combinations that a particular peptide sequence can acquire owing to its physicochemical properties.' Below this, there are two main sections: 'Basic Module' and 'Advanced Module'. The 'Basic Module' section states: 'Only calculate and list out all the possible peptide combinations.' The 'Advanced Module' section states: 'Calculates combinations upto 0.1 million along with other properties including: Molecular Weight, Net Charge, Solubility, Isoelectric Point, Hydropathy Index, 3D Model of each combinations.' At the bottom of the page, there is a footer with copyright information: '© All Rights Reserved. Biorxiv Research Institute, Dehradun (India). Created & Developed By: Bioinformatics Centre, FRI, Dehradun. Total Visits: 10'. There is also a logo for the Department of Biotechnology, Ministry of Science & Technology, India.

Figure s 1: The image indicates the main web server front page, which can be used to access both basic and advanced module for generating peptide combinations (source: <https://www.bicfri.in/pepcogen/>)

The image shows the user input page for the Peptide Combination Generator. The main heading is 'Peptide Combination Generator' with the same subtext as in Figure s 1. Below the heading, there is a section labeled 'INPUT' with a form containing 'Number of Residues', 'Select Length' (a dropdown menu), and a 'Go' button. Below the input section, there is a section labeled 'RESULT'.

Figure s 2: The image indicates the user input page for both basic and advanced module of web server (source: <https://www.bicfri.in/pepcogen/basic/>).

# Peptide Combination Generator

A tool for generating all the possible combinations that a particular peptide sequence can acquire owing to its physiochemical properties.

INPUT

Number of Residues  Select Length

Select Length

- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15
- 16
- 17
- 18
- 19
- 20
- 21

RESULT

Figure s 3: The image indicates the drop down menu to select the length of peptides ranging from 4 to 21 (source: <https://www.bicfri.in/pepcogen/basic/>).

INPUT

Number of Residues

Position 1

Position 2

Position 3

Position 4

Position 5

Position 6

Position 7

RESULT

- Acidic**  
Aspartic Acid, Asp, D  
Glutamic Acid, Glu, E
- Basic**  
Arginine, Arg, R  
Histidine, His, H  
Lysine, Lys, K
- Hydrophobic (Aliphatic)**  
Alanine, Ala, A  
Isoleucine, Ile, I  
Leucine, Leu, L  
Methionine, Met, M  
Valine, Val, V
- Aromatic**  
Phenylalanine, Phe, F  
Tryptophan, Trp, W  
Tyrosine, Tyr, Y
- Polar Uncharged**  
Asparagine, Asn, N  
Cysteine, Cys, C  
Glutamine, Gln, Q  
Serine, Ser, S  
Threonine, Thr, T
- Unique**  
Glycine, Gly, G  
Proline, Pro, P

Figure s 4: The image indicates the various positions for the peptide sequence (length 7) which have to selected for combinations with amino acids having similar physiochemical properties (source: <https://www.bicfri.in/pepcogen/basic/>).

## ===== RESULT =====

S.No.	Combination
1	DRAFSGT
2	DRAFSPPT
3	DRAFTGT
4	DRAFTPT
5	DRAFCGT
6	DRAFCPT
7	DRAFNGT
8	DRAFNPPT
9	DRAFQGT
10	DRAFQPT
11	DRAWSGT
12	DRAWSPT
13	DRAWTGT
14	DRAWTPT
15	DRAWCGT
16	DRAWCPT
17	DRAWNGT
18	DRAWNPPT
19	DRAWQGT
20	DRAWQPT
21	DRAYSGT
22	DRAYSPT
23	DRAVTGT

Figure s 5: The image indicates the result web page for basic module for calculating and listing out all the combination of the peptides (source: <https://www.bicfri.in/pepcogen/basic/>).

## ===== RESULT =====

Show 10 entries [Excel](#) [Pdf](#) Search:

S.No.	Combination	Molecular Weight (Da)	Net Charge	Solubility	Isoelectric Point (IPC Peptide)	Hydropathy Index	Model
1	DRAFSGA	722.77	0	Poor Water Solubility	6.73	Hydropathy Index	Model
2	DRAFSPA	762.83	0	Poor Water Solubility	6.73	Hydropathy Index	Model
3	DRAFTGA	736.80	0	Poor Water Solubility	6.73	Hydropathy Index	Model
4	DRAFTPA	776.86	0	Poor Water Solubility	6.73	Hydropathy Index	Model
5	DRAFCGA	738.84	0	Poor Water Solubility	6.09	Hydropathy Index	Model
6	DRAFCPA	778.90	0	Poor Water Solubility	6.09	Hydropathy Index	Model
7	DRAFNGA	749.80	0	Poor Water Solubility	6.73	Hydropathy Index	Model
8	DRAFNPA	789.86	0	Poor Water Solubility	6.73	Hydropathy Index	Model
9	DRAFQGA	763.83	0	Poor Water Solubility	6.73	Hydropathy Index	Model
10	DRAFQPA	803.89	0	Poor Water Solubility	6.73	Hydropathy Index	Model

Showing 1 to 10 of 900 entries Previous **1** 2 3 4 5 ... 90 Next

Figure s 6: The image indicates the result web page for advanced module. Each peptide combination generated is followed by its molecular weight, net charge, solubility, isoelectric point, hydropathy index and a JSmol link for generating random 3D model (source: <https://www.bicfri.in/pepcogen/advanced/>).

**RESULT**

Show 10 entries [Excel](#) [Pdf](#) Search:

S.No.	Combination	Molecular Weight (Da)	Net Charge	Solubility	Isoelectric Point (IPC Peptide)	Hydropathy Index	Model
1	AAAAA	373.44	0	Poor Water Solubility	6	Hydropathy Index	Model
2	AAAVV	401.49	0	Poor Water Solubility	6	Hydropathy Index	Model
3	AAAAL	415.52	0	Poor Water Solubility	6	Hydropathy Index	Model
4	AAAAI	415.52	0	Poor Water Solubility	6	Hydropathy Index	Model
5	AAAAM	433.55	0	Poor Water Solubility	6	Hydropathy Index	Model
6	AAAVA	401.49	0	Poor Water Solubility	6	Hydropathy Index	Model
7	AAAVV	429.54	0	Poor Water Solubility	6	Hydropathy Index	Model
8	AAAVL	443.57	0	Poor Water Solubility	6	Hydropathy Index	Model
9	AAAVI	443.57	0	Poor Water Solubility	6	Hydropathy Index	Model
10	AAAVM	461.60	0	Poor Water Solubility	6	Hydropathy Index	Model

Showing 1 to 10 of 3,125 entries Previous 1 2 3 4 5 ... 313 Next

Figure s 7: The image indicates the result web page for advanced module (source: <https://www.bicfri.in/pepcogen/advanced/>).

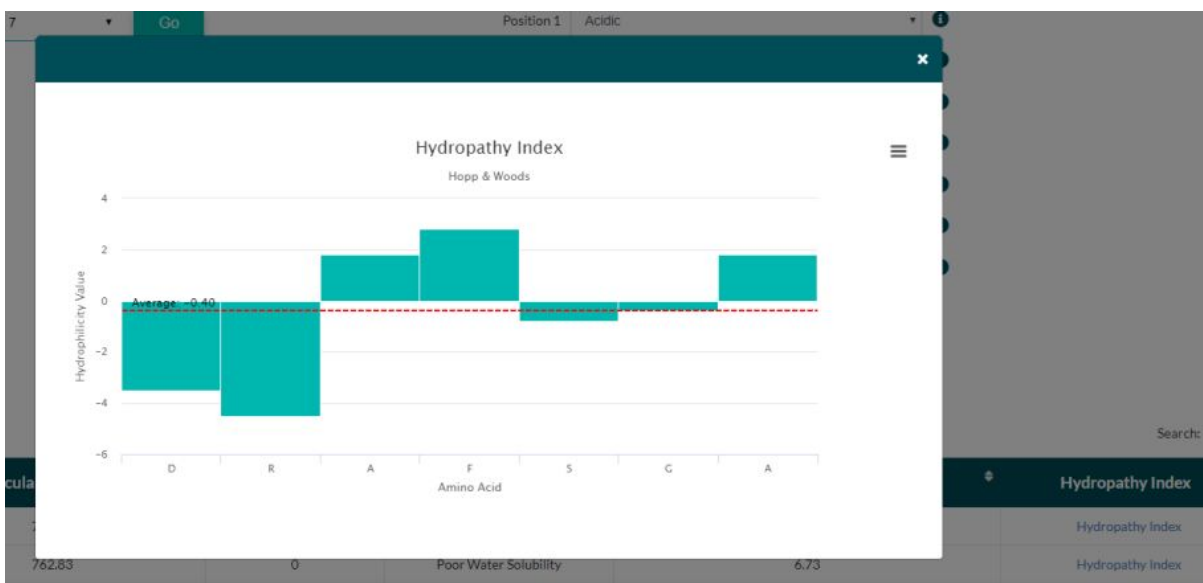


Figure s 8: The image indicates the hydropathy index of the generated peptide combination, by using the values of Hopp & Woods (source: <https://www.bicfri.in/pepcogen/advanced/>).



```

var len = (value.combination).length;
var comb = (value.combination).split("");

while (i<len) {
    if(jQuery.inArray(comb[i], pos_pKs) != -1) {
        q_pos +=1;
    }
    else if(jQuery.inArray(comb[i], neg_pKs) != -1) {
        q_neg += 1;
    }
    i++;
}
netcharge = q_pos-q_neg;

```

### Script s3:

```

//Solubility
solubility = netcharge==0?"Poor Water Solubility":"Soluble in Water";

```

### Script s4:

```

//Isoelectric point
$pK=array(
    "N_terminus"=>9.564, "K"=>10.517, "R"=>12.503, "H"=>6.018,"C_terminus"=>2.383,
    "D"=>3.887,"E"=>4.317, "C"=>8.297, "Y"=>10.071
);
$aminoacid_content=aminoacid_content($aminoacidsequence);
$charge=protein_isoelectric_point($pK,$aminoacid_content);
$result=round($charge,2);
function aminoacid_content($seq) {

$array=array("A"=>0,"R"=>0,"N"=>0,"D"=>0,"C"=>0,"E"=>0,"Q"=>0,"G"=>0,"H"=>0,"I"=>0,"L"=>
0,
    "K"=>0,"M"=>0,"F"=>0,"P"=>0,"S"=>0,"T"=>0,"W"=>0,"Y"=>0,"V"=>0);
...
return $array;
}
function protein_isoelectric_point($pK, $aminoacid_content) {
$pH=7; // pH value at start

```

```
$delta=4; // this parameter will be used to modify pH when charge!=0. The value of $delta will change during the loop
```

```
while(1) {  
    // compute charge of protein at corresponding pH (uses a function)  
    ...  
}  
return round($pH,2);  
}
```

### **Script s5:**

```
//hydropathy Index  
switch(split_val[i]) {  
    case 'A':  
        axisVal = 1.8;  
        break;  
    case 'C':  
        axisVal = 2.5;  
        break;  
    ...  
}  
highchart();
```