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

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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:

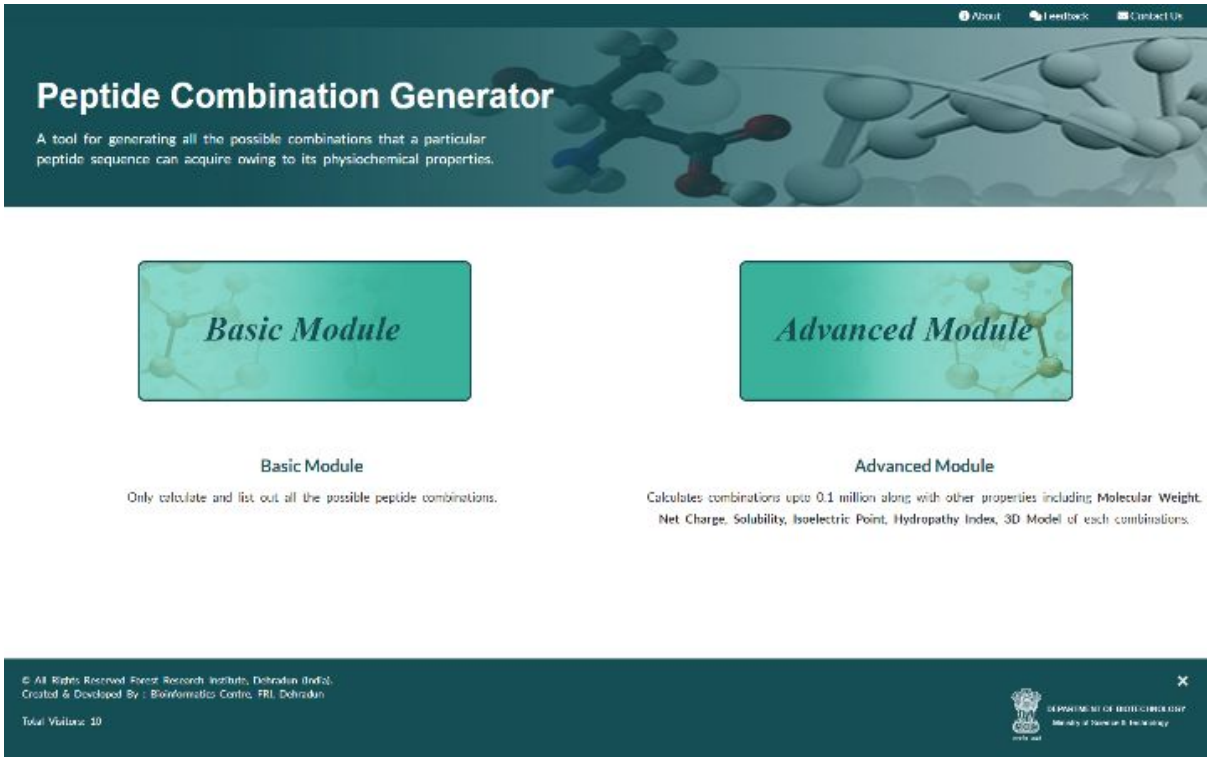

Figure s 1: The image indicates the main web server front page, which can be used to access both basic and advanced module for generating peptide combinations (source: https://www.bicfri.in/pepcogen/)

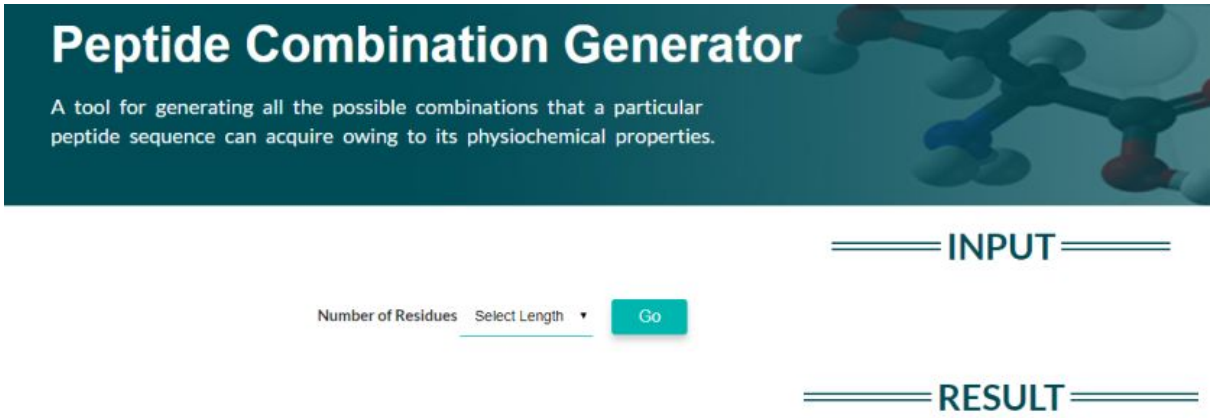

Figure s 2: The image indicates the user input page for both basic and advanced module of web server (source: https://www.bicfri.in/pepcogen/basic/).

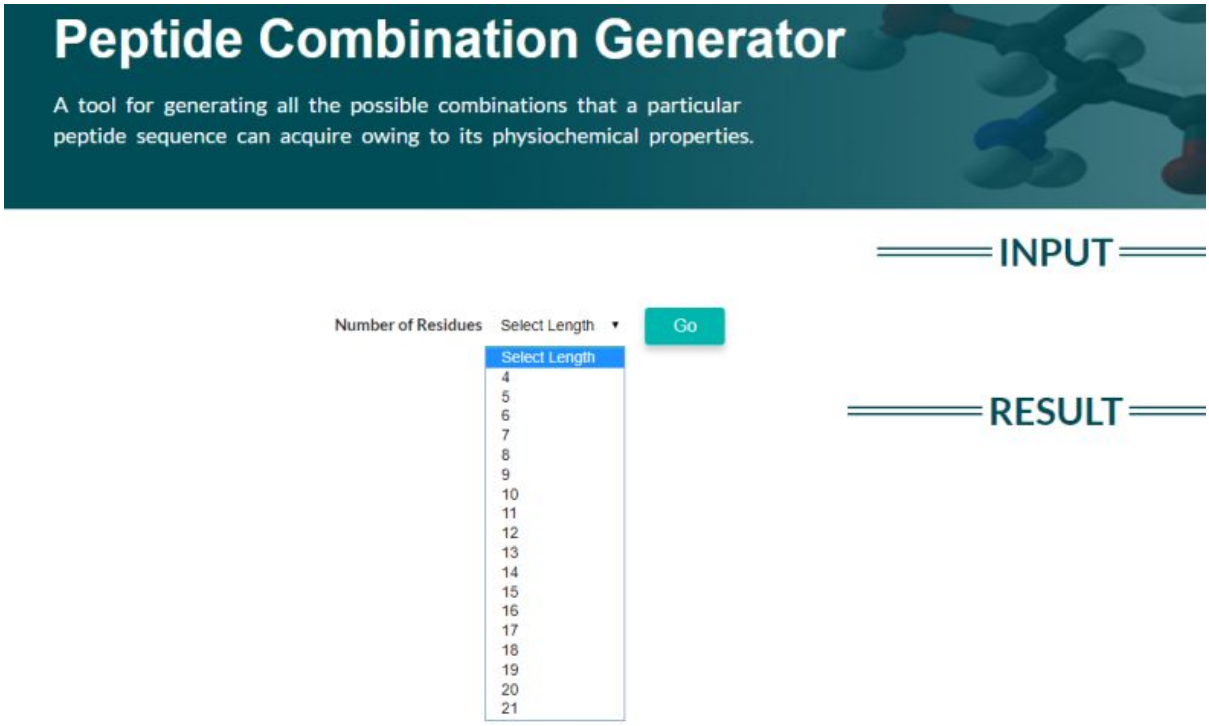

Figure s 3: The image indicates the drop down menu to select the length of peptides ranging from 4 to 21 (source: https://www.bicfri.in/pepcogen/basic/).

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	DRAFSPT
3	DRAFTGT
4	DRAFTPT
5	DRAFCGT
6	DRAFCPT
7	DRAFNGT
8	DRAFNPT
9	DRAFQGT
10	DRAFQPT
11	DRAWSGT
12	DRAWSPT
13	DRAWTGT
14	DRAWTPT
15	DRAWCGT
16	DRAWCPT
17	DRAWNGT
18	DRAWNPT
19	DRAWQGT
20	DRAWQPT
21	DRAYSGT
22	DRAYSPT
23	DRAYTGT

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/).

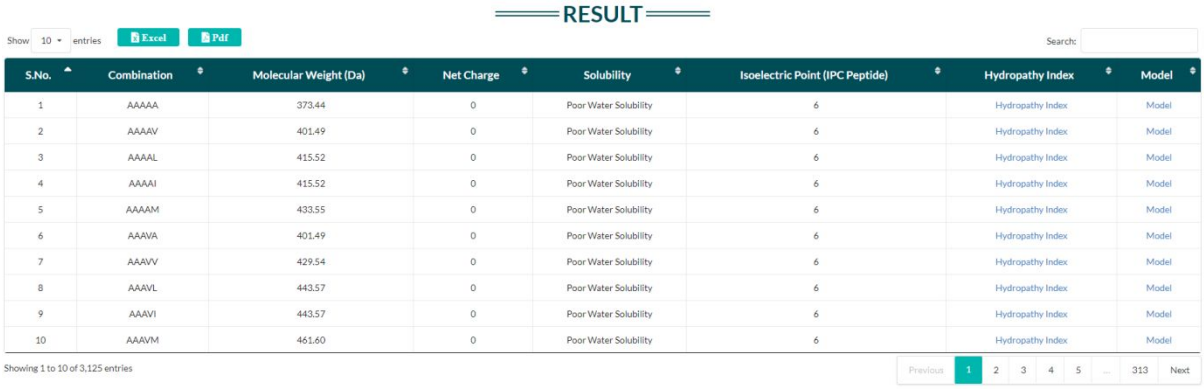

Figure s 7: The image indicates the result web page for advanced module (source: https://www.bicfri.in/pepcogen/advanced/).

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/).

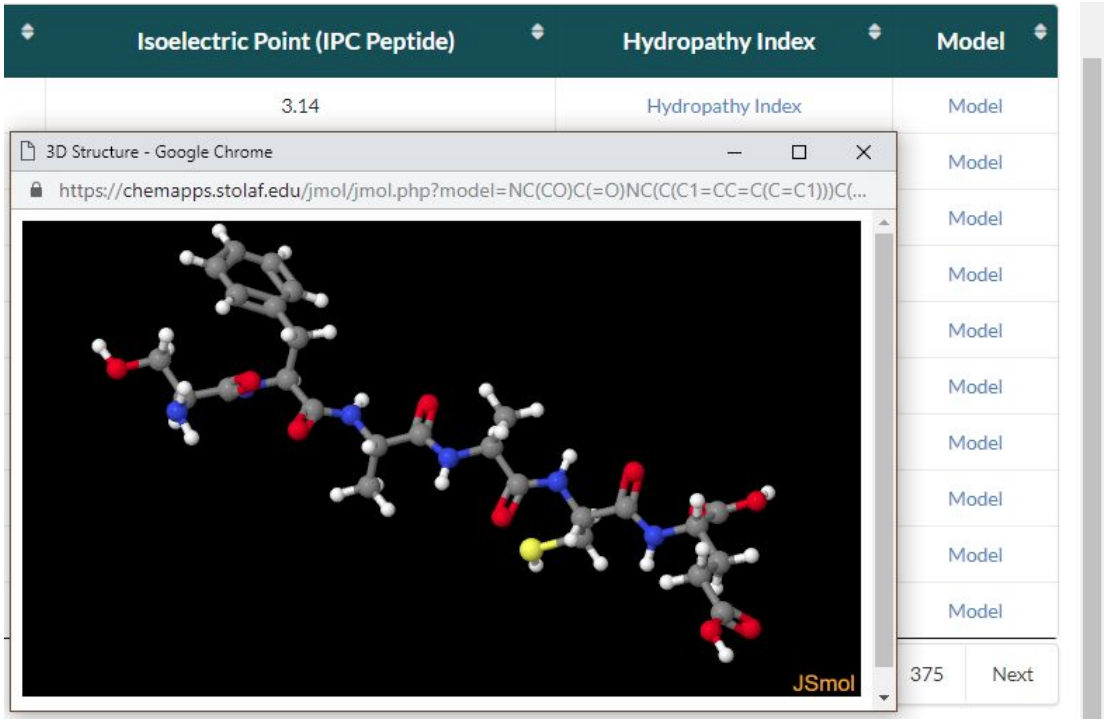

Figure s 9: The image indicates the random 3D model generated for the peptide sequence using JSmol plugin (source: https://www.bicfri.in/pepcogen/advanced/).

Script s1:

```
// Molecular Weight
switch($combination[$i]) {
        case 'A':
                $mw = 89.10;
                break;
        case 'C':
                $mw = 121.16;
                break;

        ...                             // list of other cases
        }

        bond = (combination).length-1;
        molweight = mw-(18.01528*bond);
```

Script s2:

```
// Net Charge
var pos_pKs = ['K', 'R'];
var neg_pKs = ['D', 'E'];
var q_pos = 0;
var q_neg = 0;
var i = 0;
```

```
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();
```