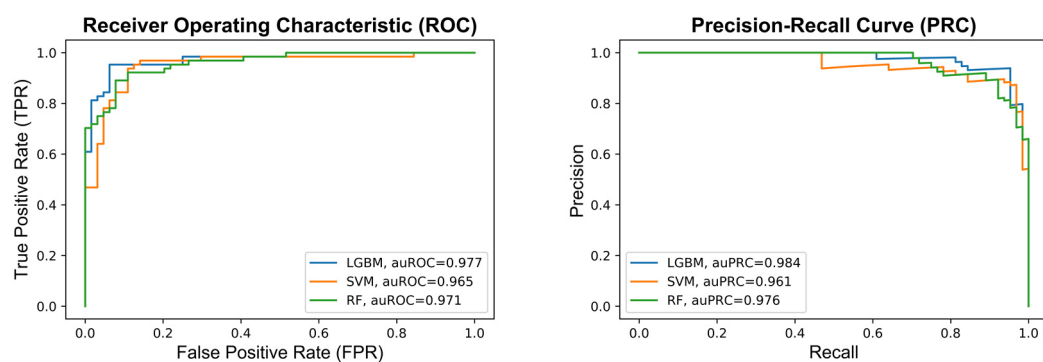


## Supplemental figures:



**Supplemental Figure S1.** The ROC curve and PRC curve of independent test of three machine learning models based on UniRep\_BiLSTM best features encoding. The ROC curve and PRC curve of independent test of three machine learning models based on UniRep\_BiLSTM top K feature encoding. For LGBM, SVM, RF, the K value is 106, 186 and 45 independently.

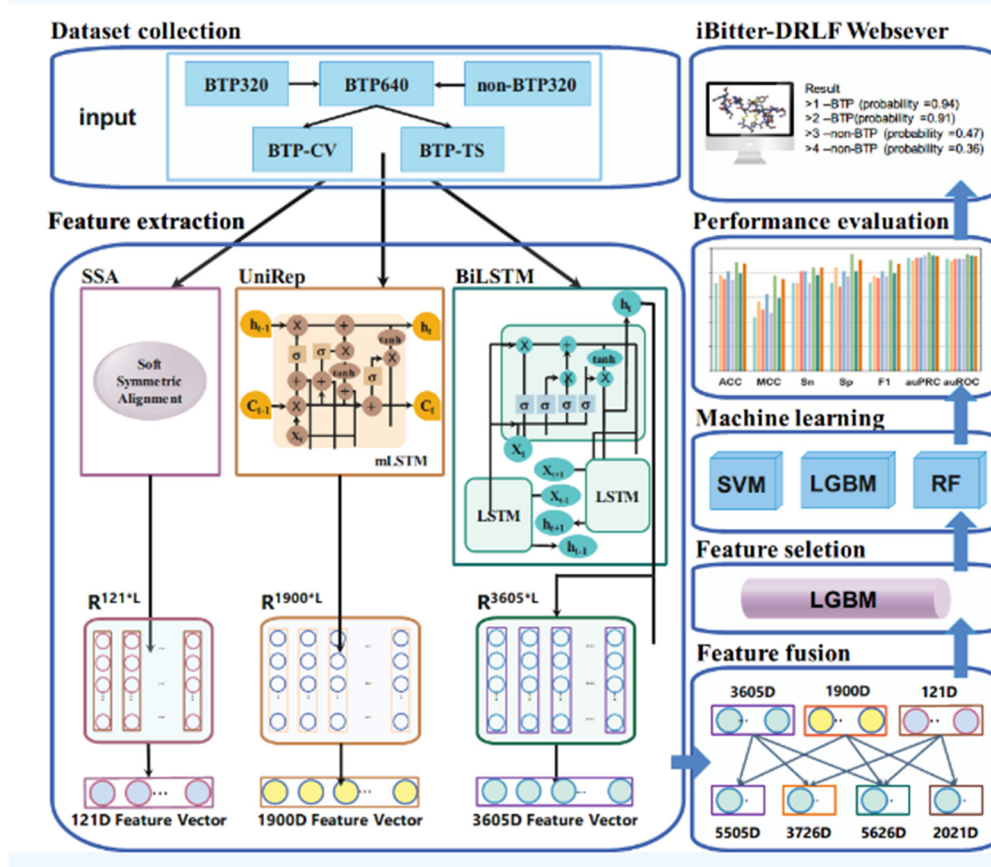
## iBitter-DRLF

A novel prediction tool for bitter peptides based on deep learning representation feature methods  
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### Introduction

A bitter taste often identifies hazardous compounds and it is generally avoided by most animals and humans. Bitterness of hydrolyzed proteins is caused by the presence of bitter peptides. To improve palatability, bitter peptides need to be identified experimentally in a time-consuming and expensive process, before they can be removed or degraded. Here, we report the development of a machine learning prediction method, *iBitter-DRLF*, which is based on a deep learning pre-trained neural network feature extraction method. It uses three sequence embedding techniques, soft symmetric alignment (SSA), unified representation (UniRep), and bidirectional long short-term memory (BiLSTM). The results showed that the use of deep representation learning greatly improves the ability of the model to identify bitter peptides, achieving accurate prediction based on peptide sequence data alone.

### Framework



**Supplemental Figure S2.** Screenshots of the iBitter-DRLF webserver. Users can access the webserver by entering <https://www.aibiochem.net/servers/iBitter-DRLF/>, which would bring us to the webpage as shown in Figure S2.

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### Input Peptides sequence in *FASTA* format and *Run*

Please input no more than 50 sequences. Otherwise, a 504 Time out error will appear. If there is a 504 error or other errors, please wait for a few minutes and refresh the page again. Or wait for several minutes and then resubmit the task.

Run

Clear

### Example

INPUT

OUTPUT\_RESULTS

```
>Seq0
VD
>Seq1
AQTQSLVYPFPGPIPNLQNIPLTQ
>Seq2
LAGNQEEE
>Seq3
VG
>Seq4
LG
>Seq5
VIFPPGR
>Seq6
VIIPFPG
>Seq7
EA
>Seq8
LLG
>Seq9
LLLL
```

SEQUENCES	BITTER PEPTIDES	CONFIDENCE
VD	YES	99.9%
AQTQSLVYPFPGPIPNLQNIPLTQ	YES	93.8%
LAGNQEEE	YES	53.5%
VG	YES	100.0%
LG	YES	93.6%
VIFPPGR	YES	97.5%
VIIPFPG	YES	96.9%
EA	YES	64.4%
LLG	YES	76.6%
LLLL	NO	87.7%

**Supplemental Figure S3.** Screenshots of the iBitter-DRLF webserver. Users can begin the prediction process by entering the query sequence into the text box and clicking the "Run" button; this step typically takes a few seconds for the server to process the task.

## ***iBitter-DRLF***

A novel prediction tool for bitter peptides based on deep learning representation feature methods

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### ***Results***

SEQUENCES	BITTER PEPTIDES	CONFIDENCE
ETWRTAPSATGQASSLLGGRLGQ	YES	96.27%
LGGIVSAVKKIVDFLG	YES	99.97%
GRKKRRQRRRGGMWVTNLRD	YES	97.48%
FAKLAKKALAKLL	YES	94.21%
KIAKVALAKLGIGAVLKVLTTGL	YES	96.78%
FLGALFKALSKLL	YES	83.27%
PLLQATLGGS	NO	74.26%
FAKLLALALKLKL	YES	97.57%
AAVPIVNLKDELLFPSWEALFSGSE	YES	98.43%
GKWKILGKLIR	NO	76.04%
GFFALIPKIISSPLFKTLLSAVGSALS	YES	93.10%
PAWRKARRWAWRMKKLAA	YES	80.51%

**Supplemental Figure S4.** Screenshots of the iBitter-DRLF webserver. After the prediction process is completed, the results are displayed on the webserver.