

Sophia Huilin Wang  
A16838155

Q1.

Name: NEDD8

Accession: NP\_006147

Species: Homo Sapiens

Function from UniProt: Ubiquitin-like protein which plays an important role in cell cycle control and embryogenesis via its conjugation to a limited number of cellular proteins, such as cullins or p53/TP53.

Q2.

Method: TBLSTN search against Hordeum vulgare ESTs

Database: Expressed Sequence Tags

Organism: Hordeum vulgare (taxid:4513)

Job Title

NP\_006147:NEDD8 [Homo sapiens]

RID

MERDN56V013 Search expires on 11-29 00:58 am [Download All](#) ▼

Program

TBLASTN [Citation](#) ▼

Database

est [See details](#) ▼

Query ID

NP\_006147.1

Description

NEDD8 [Homo sapiens]

Molecule type

amino acid

Query Length

81

Other reports

[?](#)

Filter Results

Organism only top 20 will appear ☐ exclude

[+ Add organism](#)

Percent Identity

to

E value

to

Query Coverage

to

Filter

Reset

Descriptions

Graphic Summary

Alignments

Taxonomy

Sequences producing significant alignments

Download ▼

Select columns ▼

Show  [?](#)

☒ select all 100 sequences selected

[GenBank](#) [Graphics](#)

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	AV910127 K. Sato unpublished cDNA library, cv. Akashinriki vegetative stage leaves Hordeum vulgare subsp. vulgare...	Hordeum vulgare...	99.8	99.8	80%	2e-27	78.46%	469	AV910127.1
<input checked="" type="checkbox"/>	AJ485237 S00011 Hordeum vulgare cDNA clone S0001100158E06F1, mRNA sequence	Hordeum vulgare	82.0	82.0	79%	2e-21	65.62%	240	AJ485237.1
<input checked="" type="checkbox"/>	AJ485236 S00011 Hordeum vulgare cDNA clone S0001100117C01F1, mRNA sequence	Hordeum vulgare	82.0	82.0	79%	4e-21	65.62%	300	AJ485236.1
<input checked="" type="checkbox"/>	AJ462907 S00002 Hordeum vulgare subsp. vulgare cDNA clone S0000200068G05F1, mRNA sequence	Hordeum vulgare...	82.0	82.0	79%	1e-20	65.62%	420	AJ462907.1
<input checked="" type="checkbox"/>	SFR005.F12F990624 ITEC SFR Barley Leaf Epidermis Library Hordeum vulgare subsp. vulgare cDNA clone SF.m...	Hordeum vulgare...	82.0	82.0	79%	1e-20	65.62%	431	BE437618.1
<input checked="" type="checkbox"/>	HDP08C11w HDP Hordeum vulgare subsp. vulgare cDNA clone HDP08C11, mRNA sequence	Hordeum vulgare...	84.0	143	80%	1e-20	67.19%	669	EX591222.1
<input checked="" type="checkbox"/>	AJ435026 S00002 Hordeum vulgare subsp. vulgare cDNA clone S0000200025F08F1, mRNA sequence	Hordeum vulgare...	82.8	126	79%	1e-20	65.62%	520	AJ435026.1
<input checked="" type="checkbox"/>	GCN004P12u GCN Hordeum vulgare cDNA clone GCN004P12 3-PRIME, mRNA sequence	Hordeum vulgare	82.4	82.4	79%	1e-20	65.62%	500	DN156542.1
<input checked="" type="checkbox"/>	HVSMEI0019O03f Hordeum vulgare spike EST library HVcDNA0012 (Fusarium infected) Hordeum vulgare subsp. ....	Hordeum vulgare...	82.0	124	79%	1e-20	65.62%	470	BI950248.1

Chosen match Accession AV910127.1, a 469 base pair clone from Hordeum vulgare. See below for alignment details.

AV910127 K. Sato unpublished cDNA library, cv. Akashinriki vegetative stage leaves Hordeum vulgare subsp. vulgare cDNA clone  
baak3d22 5', mRNA sequence

Sequence ID: [AV910127.1](#) Length: 469 Number of Matches: 1

Range 1: 37 to 231 [GenBank](#) [Graphics](#) [▼ Next Match](#) [▲ Previous Match](#)

Score	Expect	Method	Identities	Positives	Gaps	Frame
99.8 bits(247)	2e-27	Compositional matrix adjust.	64/65(98%)	64/65(98%)	0/65(0%)	+1
Query 1	MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQRLIYSGKQMNDEKTAADYK					60
Sbjct 37	MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQRLIYSGKQMNDEKTAADYK					216
Query 61	ILGGS	65				
Sbjct 217	I GGS	231				

Q3.

> Hordeum vulgare NEDD8 protein (sequence taken from BLAST result)  
MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQRLIYSGKQMNDEKTAADYK  
IQGGS

Name: Hordeum vulgare NEDD8 protein  
Species: Hordeum vulgare subsp. vulgare  
Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;  
Spermatophyta; Magnoliopsida; Liliopsida; Poales; Poaceae; BOP  
clade; Pooideae; Triticodae; Triticeae; Hordeinae; Hordeum.

Q4.

Details:  
A BLASTP search against NR database yielded a top hit result from Scophthalmus maximus.

Standard Protein BLAST

blastnblastpblastxtblastntblastx

BLASTP programs search protein databases using a protein query. more...

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) ClearQuery subrange

>HORDEUM VULGARE PROTEIN (SEQUENCE TAKEN FROM BLAST RESULT)  
MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQRLIYSGKQMNDEKTAADYKIQGGS

FromTo

Or, upload fileChoose FileNo file chosen

Job TitleHordeum vulgare protein (sequence taken from...  
Enter a descriptive title for your BLAST search

Align two or more sequences

Choose Search Set

DatabasesStandard databases (nr etc.): Experimental databases

CompareSelect to compare standard and experimental database

Standard

DatabaseNon-redundant protein sequences (nr)

OrganismOptionalEnter organism name or id--completions will be suggestedexcludeAdd organism  
Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown

ExcludeOptionalModels (XM/XP)Non-redundant RefSeq proteins (WP)Uncultured/environmental sample sequences

Program Selection

Algorithm

Quick BLASTP (Accelerated protein-protein BLAST)  
blastp (protein-protein BLAST)  
PSI-BLAST (Position-Specific Iterated BLAST)  
PHI-BLAST (Pattern Hit Initiated BLAST)  
DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)

Choose a BLAST algorithm

Job Title

Hordeum vulgare protein (sequence taken from...

RID

MERYTGAA013 Search expires on 11-29 01:07 am [Download All](#)

Program

BLASTP [Citation](#)

Database

nr [See details](#)

Query ID

lcl|Query\_9234185

Description

Hordeum vulgare protein (sequence taken from BLAST result)

Molecule type

amino acid

Query Length

65

Other reports

[Distance tree of results](#)
[Multiple alignment](#)
[MSA viewer](#)

Filter Results

Organism

only top 20 will appear

☐ exclude

Type common name, binomial, taxid or group name

[+ Add organism](#)

Percent Identity

to

E value

to

Query Coverage

to

Filter

Reset

Compare these results against the new Clustered nr database

BLAST

Descriptions

Graphic Summary

Alignments

Taxonomy

Sequences producing significant alignments

Download

Select columns

Show 

100

☒ select all

100 sequences selected

[GenPept](#)
[Graphics](#)
[Distance tree of results](#)
[Multiple alignment](#)
[MSA Viewer](#)

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	NEDD8 ubiquitin like modifier, like [Scophthalmus maximus]	Scophthalmus maximus	131	131	100%	9e-38	100.00%	87	<a href="#">XP_035491582.1</a>
<input checked="" type="checkbox"/>	NEDD8 ubiquitin like modifier, like [Melanotaenia boesemani]	Melanotaenia boesemani	131	131	100%	9e-38	100.00%	89	<a href="#">XP_041848872.1</a>
<input checked="" type="checkbox"/>	hypothetical protein OJAV_G00172600 [Oryzias javanicus]	Oryzias javanicus	131	131	100%	1e-37	100.00%	89	<a href="#">RVE61622.1</a>
<input checked="" type="checkbox"/>	NEDD8 [Oncorhynchus tshawytscha]	Oncorhynchus tshawytscha	130	130	100%	1e-37	100.00%	88	<a href="#">XP_024246967.1</a>
<input checked="" type="checkbox"/>	NEDD8 ubiquitin like modifier, like [Osmerus eperlanus]	Osmerus eperlanus	130	130	100%	1e-37	100.00%	88	<a href="#">XP_062337321.1</a>
<input checked="" type="checkbox"/>	NEDD8 [Coregonus clupeaformis]	Coregonus clupeaformis	130	130	100%	1e-37	100.00%	88	<a href="#">XP_041752455.1</a>

## NEDD8 ubiquitin like modifier, like [Scophthalmus maximus]

Sequence ID: [XP\\_035491582.1](#) Length: 87 Number of Matches: 1

[See 1 more title\(s\)](#) [See all Identical Proteins\(IPG\)](#)

Range 1: 1 to 65 [GenPept](#) [Graphics](#) [Next Match](#) [Previous Match](#)

Score	Expect	Method	Identities	Positives	Gaps
131 bits(329)	9e-38	Compositional matrix adjust.	65/65(100%)	65/65(100%)	0/65(0%)
Query 1	MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQQRLIYSGKQMNDKTAADYK 60				
Sbjct 1	MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQQRLIYSGKQMNDKTAADYK 60				
Query 61	IQGGS	65			
Sbjct 61	IQGGS	65			

Q5.

Re-labeled sequences for alignment:

```
>Human_NEDD8 [Homo sapiens]
MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQQRLIYSGKQMNDKTAADYKILGG
SVLHLVLALRGGGGLRQ
```

```
> Hordeum_vulgare_NEDD8(sequence taken from BLAST result)
MLIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPQQQRLIYSGKQMNDKTAADYK
IQGGS
```

```
> Triticum_dicoccoides_NEDD8
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYNIEGGS
```

```
> Zea_mays_NEDD8
MIKVKTTLTGKEIEIDIEPTDSIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYNIEGGS
```

```
> Setaria_italica_NEDD8
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYNIEGGS
```

```
> Lolium_rigidum_NEDD8
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYNIEGGS
```

### Alignment:

#### Obtained using MUSCLE (3.8) at EBI:

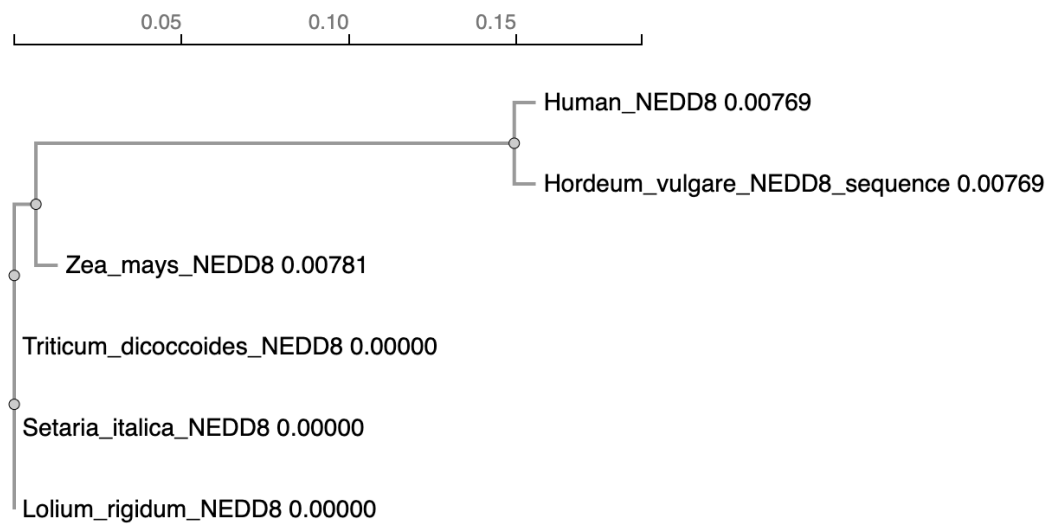
CLUSTAL multiple sequence alignment by MUSCLE (3.8)

```
Human_NEDD8
LIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPVQQRLIYSGKQMNDEKTAADYK
Hordeum_vulgare_NEDD8(sequence
LIKVKTLTGKEIEIDIEPTDKVERIKERVEEKEGIPPVQQRLIYSGKQMNDEKTAADYK
Triticum_dicoccoides_NEDD8      -
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYN
Setaria_italica_NEDD8          -
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYN
Lolium_rigidum_NEDD8           -
MIKVKTTLTGKEIEIDIEPTDTIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYN
Zea_mays_NEDD8                 -
MIKVKTTLTGKEIEIDIEPTDSIDRIKERVEEKEGIPPVQQRLIYAGKQLADDKTAKDYN
:*****.::***** *****:***: *:*** **:
```

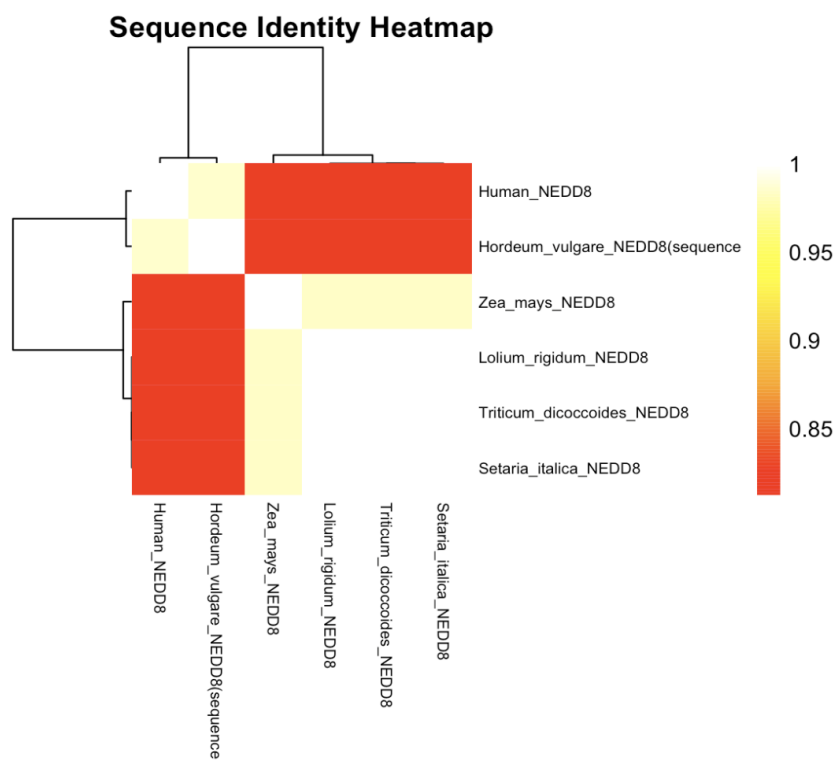
Human_NEDD8	ILGGS
Hordeum_vulgare_NEDD8(sequence	IQGGS
Triticum_dicoccoides_NEDD8	IEGGS
Setaria_italica_NEDD8	IEGGS
Lolium_rigidum_NEDD8	IEGGS
Zea_mays_NEDD8	IEGGS
	* **

Q6.

Imported the MUSCLE results to Simple Phylogeny at EBI:



Q7.



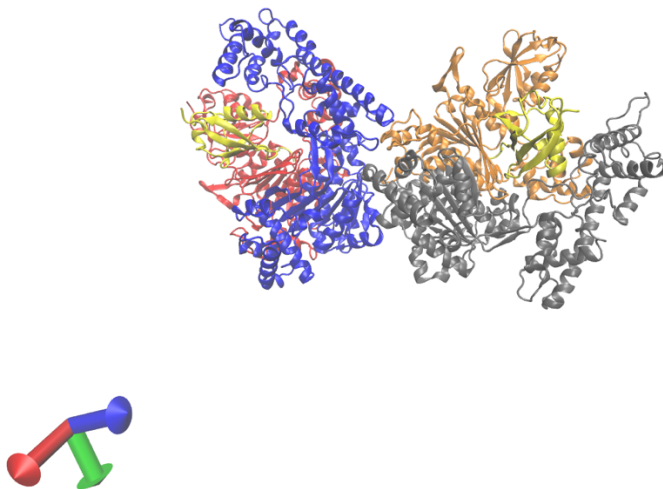
Q8.

ID	Technique	Resolution	Source	Evalue	Identity
3GZN	X-ray	3.00	Homo sapiens	2.00e-40	98.462
1BT0	X-ray	1.7	Arabidopsis thaliana	1.11e-33	83.077
3J79	EM	3.2	Plasmodium falciparum 3D7	6.04e-22	58.065

Q9.

Very likely to be similar in structure to *Hordeum vulgare* NEDD8 given the high sequence similarity (>80%). In the figure below the NEDD8 chain is colored in bright yellow and corresponds to the *Hordeum vulgare* NEDD8 subject of this report.

Using VMD:



Using Mol\*:

Conserved residues as spacefill and protein colored (ROYGBIV) by local alpha fold pLDDT quality score.



Q10.

CHEMBL details 1 Binding Assay (CHEMBL4295831); Ligand efficiency data shows a Surface Efficiency Index of 6.29, a Binding Efficiency Index of 18.78, and a Standard Value nM of 4.7.

The binding assay linked manuscript discusses the importance of Post-translational modifications (PTMs) on non-histone proteins and the association of PTMs to diseases such as cancer, inflammatory disorders, and neurodegenerative diseases.

Buuh, Z. Y., Lyu, Z., & Wang, R. E. (2018). Interrogating the Roles of Post-Translational Modifications of Non-Histone Proteins. *Journal of medicinal chemistry*, 61(8), 3239–3252. <https://doi.org/10.1021/acs.jmedchem.6b01817>