

(Solved) **QUESTION 1**

(I)

Proline can't donate an amide H bond, that's why either it breaks or kinks a helix. Its side chain interferes sterically with the backbone of the preceding turn - inside a helix, this forces a bend of about 30° in the helix's axis.

(II)

Followings are steps involved in drug design-ing:

- Discovery
- Product Characterization
- Formulation, Delivery, Packaging Development
- Pharmacokinetics & Drug Disposition
- Preclinical Toxicology Testing & IND Application
 - Acute Studies
 - Repeated Dose Studies
 - Genetic Toxicity Studies
 - Reproductive Toxicity Studies

- Carcinogenicity Studies
- Toxicokinetic Studies
- Bioanalytical Testing
- Clinical Trials
 - Phase I: Clinical Development (Human Pharmacology)
 - Phase II: Clinical Development (Therapeutic Exploratory)
 - Phase III: Clinical Development (Therapeutic Confirmatory)

(III)

ROLE OF HAIRPIN :

Role of hairpin is to enforce secure binding. It is also common to find proline residues within the actual loop portion of the β -hairpin, since this amino acid is rigid and contributes to the "turn" formation.

ROLE OF LOOPS:

Loops in Protein Structure are important not only because they interconnect secondary structural elements

and change the direction of propagation of the polypeptide chain, but they usually also harbor the active site residue.

ROLE OF TURNS:

Turns are the third of the three "classical" secondary structures with approximately one-third of all residues in Globular proteins are contained in turns that serve to reverse the direction of polypeptide chain.

(IV)

AMINO ACID IN β -SHEET

- Tyrosine
- Phenylalanine
- Tryptophan
- Threonine
- Valine
- Isoleucine

(V)

FUNCTIONS OF TIM BARREL:

- Salt bridges within TIM barrel pores are thought to contribute to the overall stability of the fold. An example of a large salt bridge network can be found in 2-deoxyribose-5-phosphate aldolase.
- The N/C-terminal and loop regions on TIM barrel proteins are capable of hosting structural inserts ranging from simple secondary structural motifs to complete domains. For Example: Oxotidine 5'-phosphate decarboxylase.
- Catalyses the interconversion of dihydroxyacetone phosphate and D-glyceraldehyde 3-phosphate at diffusion rate limit. example TIM.

(VI)

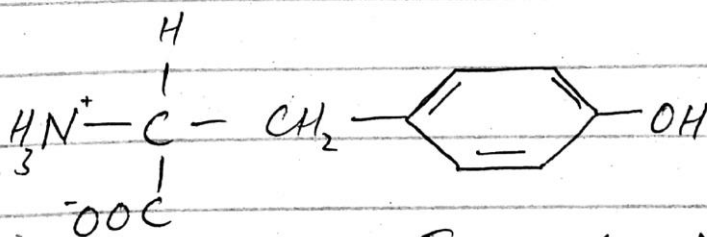
PDB vs PDB^B_{sum}:

The PDB is a key in areas of structural biology, such as structural genomics, while PDB_{sum} provides a graphic overview of PDB entries using information from other sources, such as Gene Ontology.

(VII)

STRUCTURE OF POLAR AMINO ACIDS:

The polar group consist of 10 amino acids, two are negatively charged - aspartic acid and glutamic acid, 3 have a positive charge - arginine, lysine and histidine, and 5 are uncharged - asparagine, glutamine, serine, the threonine and tyrosine.



Tyrosine (Tyr)

(VIII)

Pfam:

The Pfam database is a large collection of protein families, each represented by multiple sequence alignments and hidden Markov models (HMMs).

Pfam also generates higher-level groupings of related entries, known as clans. A clan is a collection of Pfam entries which are related by similarity of sequence, structure or profile-HMM.

Finding data in various ways:

- Analyse your protein sequence for Pfam matches
- View Pfam annotation and alignments
- See groups of related entries
- Look at the domain organisation of a protein sequence.
- Find the domains on a PDB structure

(IX)

JELLY ROLL MOTIF VS GREEK KEY MOTIF:

Jelly roll motif describes a particular topology for arranging eight strands into an antiparallel β -sheet that is frequently found in protein structures. ~~The name~~

The Greek key motif describes a particular topology for arranging four β -strands into an antiparallel β -sheet in protein structure. A common domain structure in proteins is the Greek key β -barrel, a type of antiparallel β -barrel, where two Greek key β -sheets fold together to form an eight-stranded antiparallel β -barrel.

(X)

PROMOTER & REGULATORY BOXES:

Promoter is a sequence of DNA to which proteins bind that initiate transcription of a single RNA from the DNA downstream of it. Promoters are located near the transcription start sites of genes, upstream on the DNA. Promoters can be about 100-1000 base pairs long. A regulatory box has sequence which is a segment of a nucleic acid molecule which is capable of increasing or decreasing the expression is an essential feature of all living organisms and viruses.

Question 2

(PART 1)

Features of Protein Primary Structure

- The primary structure of a protein refers to the sequence of amino acids in the polypeptide chain.
- The primary structure is held together by polypeptide bonds that are made during the process of protein biosynthesis.
- The primary structure of a protein is determined by the gene corresponding to the protein.
- Protein gets all its properties from its primary structure.
- In primary structure, all amino acids have the alpha Carbon bonded to a Hydrogen Atom, Carboxyl Group & an Amino Group.

(PART 2)

Tunnels in Protein:

Tunnels are access paths connecting the interior of molecular systems with the surrounding environment. The presence of tunnels in proteins influences their reactivity, as they determine the nature and intensity of the interaction that these proteins can take part in.

Cavities in Proteins:

Protein cavities are specific regions on the protein surface where ligands may bind. Such cavities are putative binding sites of proteins for ligands. Usually, cavities correspond to voids, pockets, and depressions of molecular surfaces.

Active Sites of Proteins:

The active site is the region of an enzyme where substrate molecules bind and undergo a chemical reaction. The active site consists of amino acids residues that catalyse a reaction of that substrate.

Allosteric Site of Protein:

The allosteric site is the active site of an adjoining protein subunit. The binding of oxygen to one subunit induces a conformational change in that subunit that interacts with the remaining active sites to enhance their Oxygen affinity.

TASK 1

a. Sequence 1: PEX5

The screenshot shows a web browser with three tabs: 'justbio software', 'Translator | JustBio - (adsbygoog)', and 'Nucleotide BLAST: Search nucle...'. The main window displays the NCBI Nucleotide database page for 'Dryopteris fragrans CHI (CHI) mRNA, partial cds' (GenBank: KP658975.1). The FASTA sequence is shown, and various analysis options are available on the right, including 'Run BLAST', 'Pick Primers', and 'Highlight Sequence Features'. Below this, the JustBio Translator tool is shown with the same sequence input, and the NCBI BLAST results page is displayed, showing the sequence alignment and filter results.

NCBI Nucleotide Database Page:

Search: Nucleotide
Advanced
Help

COVID-19 is an emerging, rapidly evolving situation.
Get the latest public health information from CDC: <https://www.cdc.gov/coronavirus>
Get the latest research from NIH: <https://www.nih.gov/coronavirus>
Find NCBI SARS-CoV-2 literature, sequence, and clinical content: <https://www.ncbi.nlm.nih.gov/sars-cov-2/>

FASTA
Send to: Change region shown
Customize view

Dryopteris fragrans CHI (CHI) mRNA, partial cds
GenBank: KP658975.1
GenBank Graphics

>KP658975.1 Dryopteris fragrans CHI (CHI) mRNA, partial cds
AAGAGTATCAACCGTCTCTTCTGCTGTGTACGCTGATGAACGATCTCAAGATAGCTTGTAGCA
AGTACACTCAACATGTGGCTGGGACTTGCAGGAAGAGCTTTTATGATGATATCTTGGATCAGA
TTTCACTTGAATGTGAGGCTGATGCTGTGTACGAGCAATAAATCGCTTCGTCGAGATGCTTT
GAAGATTCTATTGGGAGCGAATAAGAAATTAATGCTCAGCAATCGCTCTCTTCTCAAGCTTCA
CATCATTTCAAGGATGACATCAAGCTGCTCAGGGGCAATATAGACATAACCGGATCATGSCCA
TGTCTTCAACAAAAATCAATGACATGGAATCTGGATCTGTGCAAGCCCACTCTGTGTGCTCGTTT
ATGGATCTCTACATTGGGAGGATCCATTGA

Analyze this sequence
Run BLAST
Pick Primers
Highlight Sequence Features
Find in this Sequence

Related information
Protein
Taxonomy

Activate Windows
Go to Settings to activate Windows.

Recent activity
Turn Off Clear

JustBio Translator
Bioinformatics at the tip of your fingers

Hosted Tools
Software
CV Bank
Contact
Register
My Account
About
Advertise

Login
Password
Email
81052
registered users
www.Cellbiol.com
Resources for Molecular and Cell Biologists

Translator

TRANSLATOR Input Form
Type or paste your DNA sequence:

TTTCAACTTGACTGTGAGGCTAGTAATCGTGTACGAGCAATAAAATCGGTCGCGAAGTGCATTT
GAAGATTCTATTGGGAGCGAATAAGAAATTAATGCTCAGCAATCGCTCTCTTCTCAAGCTTCA
CATCATTTCAAGGATGACATCAAGCTGCTCAGGGGCAATATAGACATAACCGGATCATGSCCA
TGTCTTCAACAAAAATCAATGACATGGAATCTGGATCTGTGCAAGCCCACTCTGTGTGCTCGTTT
ATGGATCTCTACATTGGGAGGATCCATTGA

Codon table: Standard Genetic Code

1 Phase
from 1
from ATG
from ATA (note: use T not U)

3 Phases
(3 phases from 5' end of DNA template)

6 Phases
(3 phases from both orientations on DNA template)

Output formatting options
Single Phase Translation Options (1 Phase):
☐ Space between codon
☐ AA letter displayed on middle of codon (otherwise will be aligned to first nucleotide of codon)

General Options:
Number of residues per line: 60 (use multiples of 3 please)

Translate Clear

NCBI BLAST Results Page:

BLAST® » blastn suite » results for RID-KU28T9CC01R
Home Recent Results Saved Strategies Help

< Edit Search Save Search Search Summary

Job Title KP658975.1 Dryopteris fragrans CHI (CHI) mRNA,...

RID KU28T9CC01R Search expires on 08-20 19:12 pm Download All

Program BLASTN Citation

Database nt See details

Query ID lcl|Query_42183

Description KP658975.1 Dryopteris fragrans CHI (CHI) mRNA, partial cds

Molecule type dna

Query Length 452

Other reports Distance tree of results MSA viewer

How to read this report? BLAST Help Videos Back to Traditional Results Page

Filter Results

Organism only top 20 will appear exclude
Type common name, binomial, taxid or group name
+ Add organism

Percent Identity E value Query Coverage
to to to
Filter Reset

Descriptions Graphic Summary Alignments Taxonomy

Sequences producing significant alignments Download Manage Columns Show 100

☒ select all 1 sequences selected GenBank Graphics Distance tree of results

Description	Max Score	Total Score	Query Cover	E value	Per. Identity	Accession
<input checked="" type="checkbox"/> Dryopteris fragrans CHI (CHI) mRNA, partial cds	835	835	100%	0.0	100.00%	KP658975.1

Feedback

b. Sequence 2: PIK3CA

justbio software] - Yahoo Search X Translator | JustBio - (adsbygoo) X Dryopteris fragrans flavanone-3- NCBI Blast:KP658976.1 Dryopter

https://blast.ncbi.nlm.nih.gov/Blast.cgi

BLAST® » blastn suite » results for RID-KU2RYCJ014

Home Recent Results Saved Strategies Help

How to read this report? BLAST Help Videos Back to Traditional Results Page

Job Title KP658976.1 Dryopteris fragrans flavanone-3-hydroxylase

RID KU2RYCJ014 Search expires on 08-20 19:20 pm Download All

Program BLASTN Citation

Database nt See details

Query ID lcl|Query_64587

Description KP658976.1 Dryopteris fragrans flavanone-3-hydroxylase (F3) ...

Molecule type dna

Query Length 693

Other reports Distance tree of results MSA viewer

Filter Results

Organism only top 20 will appear exclude

Type common name, binomial, taxid or group name

+ Add organism

Percent Identity E value Query Coverage

to to to

Filter Reset

Descriptions Graphic Summary Alignments Taxonomy

Sequences producing significant alignments

Download Manage Columns Show 100

select all 1 sequences selected

Description	Max Score	Total Score	Query Cover	E value	Per Ident	Accession
Dryopteris fragrans flavanone-3-hydroxylase (F3H) mRNA, partial cds	1280	1280	100%	0.0	100.00%	KP658976.1

Activate Windows Go to Settings to activate Windows.

justbio software] - Yahoo Search X Translator | JustBio - (adsbygoo) X ncbi - Yahoo Search Results Yaho Dryopteris fragrans CHI (CHI) mli X

https://www.justbio.com/index.php?page=translator

Translation from: ATG

Codon View

ATG AAA CGA GTC TCA AAG ATA AGC TTG GTA GCA AGT ACA CTC
AAG AGT TGG CTG GGA ACT TGC AAG AAA AGA AGT GTT TTT ATG
ATG ATA TTC TGG CAT CAG ATT TCA ACT TGA CTG TGA GGC TAG
TAA TCG TGT ACG GAC GAA TAA AAA TCG GTT CCG TGC GAA GTG
CAT TTG AAG ATT CTA TTG GCA GGC GAA TAA AGA AAT TTA GTG

Translated Protein Sequence

MKRVSKLSVASTLNSWLOTCKKTSLFMMIFWHQIST'LQ""SCTDE*KSVPCE
VHLKLLAAE*RNVAQTALFFTAHHYSRMTSSCLRGQL*TPGIMAMFLOQ
SMTYNLGLDKAHSVARLWISLGRHLX

Formatted output:

1 - AAGAGTATACCGTCTACTCTTTCGGTGTGTACGCTGATGAACGAGTCTCAAGATAAG - 68
1 - M K R V S K I S - 8
61 - CTTGTGATCAAGTACTCAACAGTTGGCTGGAGCTTGCAGGAAAAGAGTCTTTTAT - 128
9 - L V A S T L N S W L G T C K K T S L F M - 28
121 - GATGATATTCTGGCATCAGATTTCACCTGACTGTGAGGCTAGTAATCGTGTGACGAG - 188
29 - M I F M H Q I S T * L * G * * S C T D E - 48
181 - ATAAAGATCGTTCCGTGCGAGTGCATTGAAGATTCTATGGCAGCCGAATAAGAAA - 248
49 - * K S V P C E V H L K I L L A A E * R N - 68
241 - TTATGGCTCAGACAACTCCCTCTTTCACAGCTTCACATATTCAAGGATGAC - 308
69 - L V A Q T I A L F F T A S H H Y S R M T - 88
301 - ATCAAGCTGCTCAGGGACAAATTAGACATACCCGACATCATGCGCCATTCTTACA - 368
89 - S S C L R G Q L * T * P G I M A M F L Q - 108
361 - ACAAGAAATCAATGACATGCACTGGATCTGTGCAAGCCCACTTGTGTGCTGCTTT - 428
109 - Q K S M T M N L D L C K A H S C V A R L - 128
421 - ATGGATCTCTACATTGGGAGGATCCATTGA - 452
129 - M I S T L G R I H L X - 148

Activate Windows Go to Settings to activate Windows.

justbio software] - Yahoo Search X Translator | JustBio - (adsbygoo) X Dryopteris fragrans flavanone-3- NCBI Blast:KP658976.1 Dryopter

https://www.ncbi.nlm.nih.gov/nuccore/KP658976.1?report=fasta

NCBI Resources How to Sign in to NCBI

Nucleotide Nucleotide Search

Advanced Help

COVID-19 is an emerging, rapidly evolving situation.
Get the latest public health information from CDC: https://www.coronavirus.gov/
Get the latest research from NIH: https://www.nih.gov/coronavirus
Find NCBI SARS-CoV-2 literature, sequence, and clinical content: https://www.ncbi.nlm.nih.gov/sars-cov-2/

FASTA

Send to Change region shown Customize view

Dryopteris fragrans flavanone-3-hydroxylase (F3H) mRNA, partial cds

GenBank: KP658976.1

GenBank Graphics

>KP658976.1 Dryopteris fragrans flavanone-3-hydroxylase (F3H) mRNA, partial cds
TG66807TCTTCAGGTGTGTGCAACATGTGTCTCCGCCGAGATTCTGGAGCAGATGATGATGTGGGCG
CCACATTTTTCGCTCCCTCCATGAGAGAGAGCTTTATGCTCTGCAACCTGGGTGTCTGCTGCGCGA
AGGATATGCGCATCGTATGCTGTCAGAGATGACCAAGCTCTTGAATGGGAGGACTCTTTGACCATCA
ACCTCTCCCTCTTCCGAGAAACCTGAGACATGCGCCACACACCCAGCATACAGGCAACCATCA
TCSATACAGTAAAGCAGATGAGCTTTTAAAGACAACTACTGGCATTTGATTTGCGAAGCTCTGGGCT
GAGGCTCTTATATTGAAGTGCATTGAGAGCTTATCAAAATGTGTGTTAAATATTATCTCTCT
TGTCACAGCAGAACTCACTAGGTGTCAGTCTCATGATCTTGGGAGGACATGATGATGATGATGAT
AAGATGAGTGAAGAGGTTTGCAGTGTGTATAGATGCAATTTGGTGTGCGTGCACCAATTCATGATG
CTTGGTTGAGACTTGGAGACCAATACAGATATTGAGCAATGGGAGGTGCAAAATATTGAGCATGCT
GCTGTGGTAAACAAGAGAGAGGATTTCTGTGGCACTTTTATGATCACTCAAGGAA

Analyze this sequence Run BLAST Pick Primers Highlight Sequence Features Find in this Sequence

Related information Protein Taxonomy

Activate Windows Go to Settings to activate Windows.

Recent activity Turn Off Clear

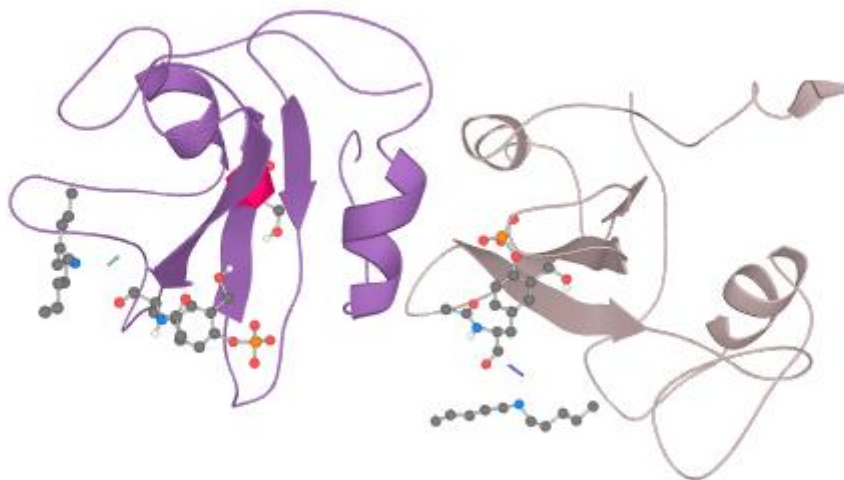
c. Sequence 3: PIK3CB

[illegible]

Task 2

PDB ID: 1A09

<https://mole.upol.cz/online/QJMLegEDPU69YqqkeyAmYw>



- Cavities (7)

All

None

☐ 1, Volume: 3216 Å³

☐ 2, Volume: 781 Å³

☐ 3, Volume: 639 Å³

☐ 4, Volume: 371 Å³

☐ 5, Volume: 274 Å³

☐ 6, Volume: 222 Å³

☐ 7, Volume: 117 Å³

- Voids (2)

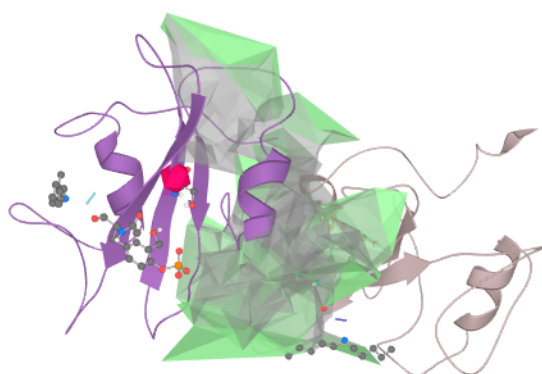
All

None

☐ 1, Volume: 185 Å³

☐ 2, Volume: 63 Å³

Help ?



- Cavities (7)

☒ 1, Volume: 3216 Å³

☐ 2, Volume: 781 Å³

☐ 3, Volume: 639 Å³

☐ 4, Volume: 371 Å³

☐ 5, Volume: 274 Å³

☐ 6, Volume: 222 Å³

☐ 7, Volume: 117 Å³

- Voids (2)

☐ 1, Volume: 185 Å³

☐ 2, Volume: 63 Å³

Submission settings

Submissions

Channels

► Active Atoms/Residues

