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Roll No: BS21B019

Bioinformatics

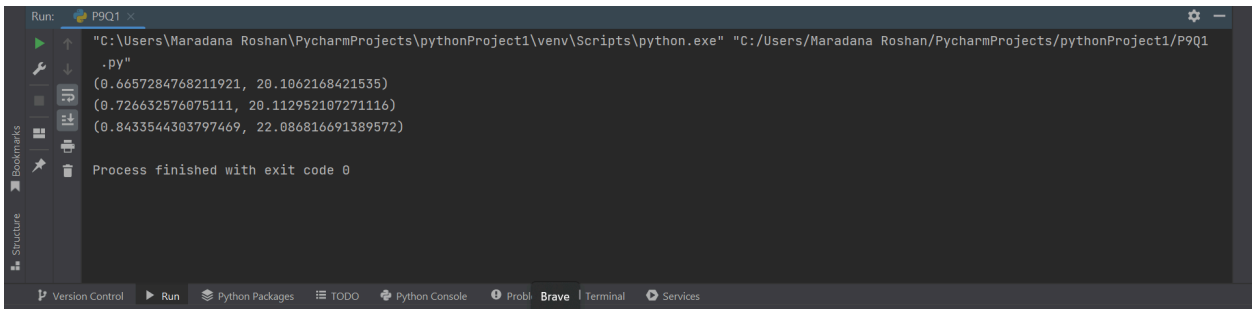
Practical 8

1. Identify the pair of sequences which are close to each other using Hamming and Euclidean distance methods.
(i)AMENLNMDLLYMAAAVMMGLAAIGAAIGIGILGGKFLEGAARQPDLIPLLRTQFFIVMGLVD AIPMIAVG LGLYVMFAVA
(ii)AADVSAAVGATGQSGMTYRLGLSWDWDKSWWQTSTGRLTGYWDAGYTYWEGGDEGA GKHSLSFAP VFVYEFAGDSIKPFIEAGIGVAAFSGTRVGDQNLGSSLNFEDRIGAGLKFANGQSVGVRAIHYS NAGLKQPN DGIESYSLFYKIPI
(iii)MALLPAAPGAPARATPTRWPVGCFNRPWTKWSYDEALDGIKAAGYAWTGLLTASKPSLH HATATPEY LAALKQKSRHAA

```
import math

def calculate_composition(sequence):
    composition = {}
    seq_length = len(sequence)
    for base in set(sequence):
        composition[base] = sequence.count(base) / seq_length
    return composition

def hamming_distance(seq1, seq2):
    composition_seq1 = calculate_composition(seq1)
    composition_seq2 = calculate_composition(seq2)

    seq_union =
set(composition_seq1.keys()).union(set(composition_seq2.keys()))

    distance = 0
    euclidean_distance = 0

    for base in seq_union:
        mod = abs(composition_seq1.get(base, 0) -
composition_seq2.get(base, 0))
        distance += mod
        euclidean_distance += mod ** 2

    euclidean_distance = math.sqrt(euclidean_distance) * 100
    return distance, euclidean_distance
```

```
seq_1 =
"AMENLNMDLLYMAAAVMMGLAAIGAAIGIGILGGKFLEGAARQPDLIPLLRTQFFIVMGLVDAIPMIAVGLGL
YVMFAVA"
seq_2 =
"AADVSAAVGATGQSGMTYRLGLSWDWDKSWWQTSTGRLTGYWDAGYTYWEGGDEGAGKHSLSFAPVFVYEFAG
DSIKPFIEAGIGVAAFSGTRVGDQNLGSSLNFEDRIGAGLKFANGQSVGVRAIHYSNAGLKQPNDGIESYSLFY
KIPI"
seq_3 =
"MALLPAAPGAPARATPTRWPVGCFNRPWTKWSYDEALDGIKAAGYAWTGLLTASKPSLHHATATPEYLAALKQ
KSRHAA"

print(hamming_distance(seq_1, seq_2))
print(hamming_distance(seq_2, seq_3))
print(hamming_distance(seq_1, seq_3))
```

Output:



2. Get the non-redundant sequences of beta barrel membrane proteins with sequence identities of less than 40%, 50%, 75% and 90% using CD-HIT

- Downloaded the manually done CD HIT sequences using MobaXTerm & followed the instructions given in the question

-

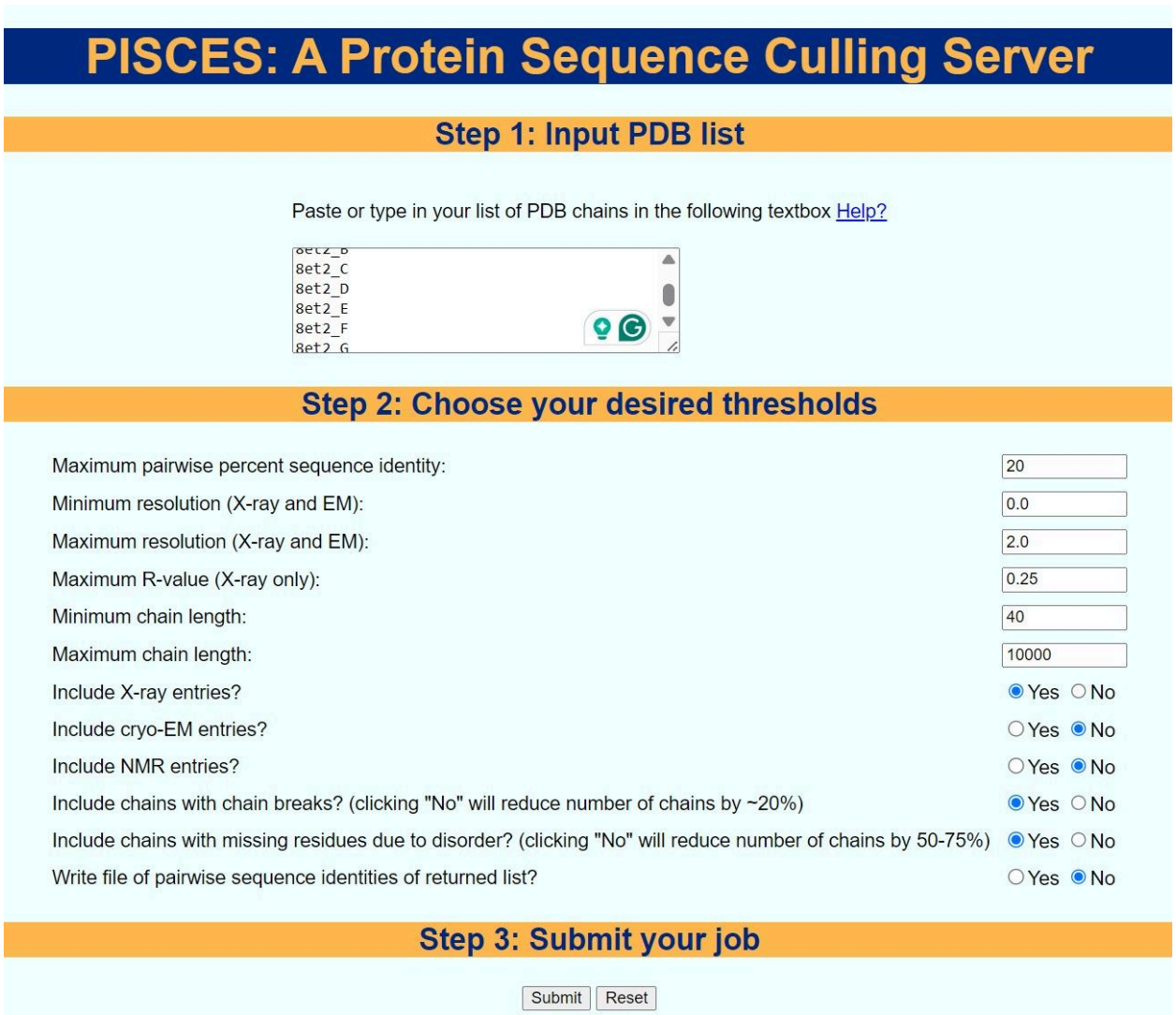
Percentage identity	Total no.of clusters
40%	239
50%	264
75%	329
90%	369

3. Get the non-redundant sequences of the same type of proteins with sequence identities of less than 20%, 30%, 40% and 50% using PISCES (https://dunbrack.fccc.edu/pisces/)

Ans)

- Ran PISCES and from the results obtained we can see the chains representing each cluster
- Percentage identity — Total no.of clusters

Percentage identity	Total no.of clusters
20%	31
30%	39
40%	42
50%	47



PISCES: A Protein Sequence Culling Server

Your representative PDB list will be generated based on the following criteria:

Sequence percentage identity	<= 20%
Sequence chain length	40 ~ 10000
Resolution	0.0 ~ 2.0
R-factor value	0.25
X-ray entries	include
EM entries	exclude
NMR entries	exclude
Allow chain breaks	yes
Allow disorder	yes
Print seqids	no

In order to send you the result, please fill out following information:

User Name: Roshan
Email address: bs21b019@smail.iitm.ac.in
Institution: Indian Institute of Technolog

Submit Reset

- First get the codes of the redundant sequences of beta barrel membrane proteins and paste them in the PISCES website
- Set the sequence identity to 20%,30%,40% and 50% and obtain the results and count the no.of clusters

4. Compare the results obtained with the cut-offs 40% and 50%.

cullpdb_pc40.0_res0.0-2.0_len40-1

File Edit View

PDBchain	len	method	resol	rfac	freerfac
3GP6A	163	XRAY	1.4	0.173	0.208
2FGQX	332	XRAY	1.45	0.15	0.171
5FVNA	342	XRAY	1.45	0.156	0.183
3SZVA	401	XRAY	1.45	0.184	0.198
4RJWA	429	XRAY	1.52	0.151	0.168
6EHBA	320	XRAY	1.55	0.172	0.199
4RLCA	175	XRAY	1.6	0.191	0.229
1QJPA	171	XRAY	1.65	0.155	0.198
6EHDA	325	XRAY	1.66	0.188	0.214
5AZPA	455	XRAY	1.69	0.161	0.18
3PGUA	427	XRAY	1.7	0.168	0.18
4D5BA	339	XRAY	1.702	0.168	0.19
5DL7A	419	XRAY	1.75	0.169	0.191
8PZ4A	479	XRAY	1.77	0.19	0.234
2PORA	301	XRAY	1.8	0.186	NA
1YC9A	442	XRAY	1.8	0.19	0.221
2WJRA	214	XRAY	1.8	0.195	0.23
3QRAA	157	XRAY	1.801	0.2	0.228
6HCPA	706	XRAY	1.83	0.157	0.177
7VU2A	435	XRAY	1.85	0.174	0.197
6I96A	677	XRAY	1.85	0.183	0.219
2X55A	293	XRAY	1.85	0.196	0.209
6TZKA	451	XRAY	1.852	0.165	0.183
4E1SA	242	XRAY	1.855	0.178	0.233
7AHLA	293	XRAY	1.89	0.199	0.257
3PRNA	289	XRAY	1.9	0.169	0.19
5MDRA	352	XRAY	1.9	0.172	0.183
5FOKA	730	XRAY	1.9	0.19	0.211
3FIDA	296	XRAY	1.9	0.193	0.23
4FQEA	222	XRAY	1.93	0.215	0.248
6QGWA	411	XRAY	1.938	0.191	0.23
6QGWB	123	XRAY	1.938	0.191	0.23
2GUFA	594	XRAY	1.95	0.191	0.225
2VDFA	253	XRAY	1.95	0.227	0.272
6FOKA	723	XRAY	1.97	0.211	0.232
3AEHA	308	XRAY	2.0	0.177	0.222
2GR8A	99	XRAY	2.0	0.193	0.215
2ERVA	150	XRAY	2.0	0.2	0.233
1KMOA	774	XRAY	2.0	0.207	0.245
6E4VA	693	XRAY	2.0	0.208	0.235
1XKWA	665	XRAY	2.0	0.222	0.242
7PGEB	215	XRAY	2.0	0.222	0.253

Ln 1, Col 1 | 1,938 characters

cullpdb_pc50.0_res0.0-2.0_len40-1

File Edit View

PDBchain	len	method	resol	rfac	freerfac
3GP6A	163	XRAY	1.4	0.173	0.208
2FGQX	332	XRAY	1.45	0.15	0.171
5FVNA	342	XRAY	1.45	0.156	0.183
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2PORA	301	XRAY	1.8	0.186	NA
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7VU2A	435	XRAY	1.85	0.174	0.197
6I96A	677	XRAY	1.85	0.183	0.219
2X55A	293	XRAY	1.85	0.196	0.209
6TZKA	451	XRAY	1.852	0.165	0.183
4E1SA	242	XRAY	1.855	0.178	0.233
7AHLA	293	XRAY	1.89	0.199	0.257
3PRNA	289	XRAY	1.9	0.169	0.19
5MDRA	352	XRAY	1.9	0.172	0.183
5FOKA	730	XRAY	1.9	0.19	0.211
3FIDA	296	XRAY	1.9	0.193	0.23
1QJ8A	148	XRAY	1.9	0.204	0.246
4FRXA	437	XRAY	1.9	0.214	0.247
4FQEA	222	XRAY	1.93	0.215	0.248
6QGWA	411	XRAY	1.938	0.191	0.23
6QGWB	123	XRAY	1.938	0.191	0.23
5FP1A	718	XRAY	1.94	0.158	0.181
2GUFA	594	XRAY	1.95	0.191	0.225
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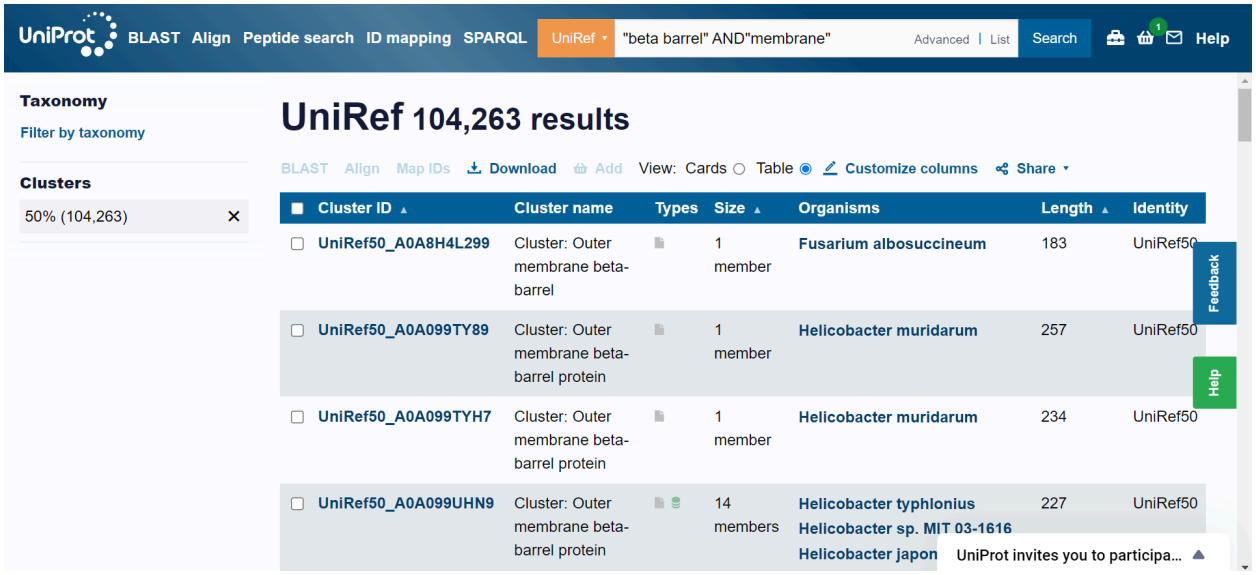
6E4VA	693	XRAY	2.0	0.208	0.235
1XKWA	665	XRAY	2.0	0.222	0.242
7PGEB	215	XRAY	2.0	0.222	0.253

Ln 7, Col 45 | 2,118 characters | 70% | Unix (LF) | UTF-8

No.of chains with 40% identity are 42
No.of chains with 50% identity are 47

5. Extract the data with the cut-off of 50% from Uniprot and compare with CD-HIT and PISCES.



i) First go to Uniprot
ii) Change the seach setting to UniRef
iii) Search “beta barrel”AND”membrane”
iv) Select the 50%sequence identity

No.of clusters with cutoff of 50% in
CD-HIT : 264
PISCES: 47
UniProt: 104,263