**Day 2:**

**Gene Annotation**

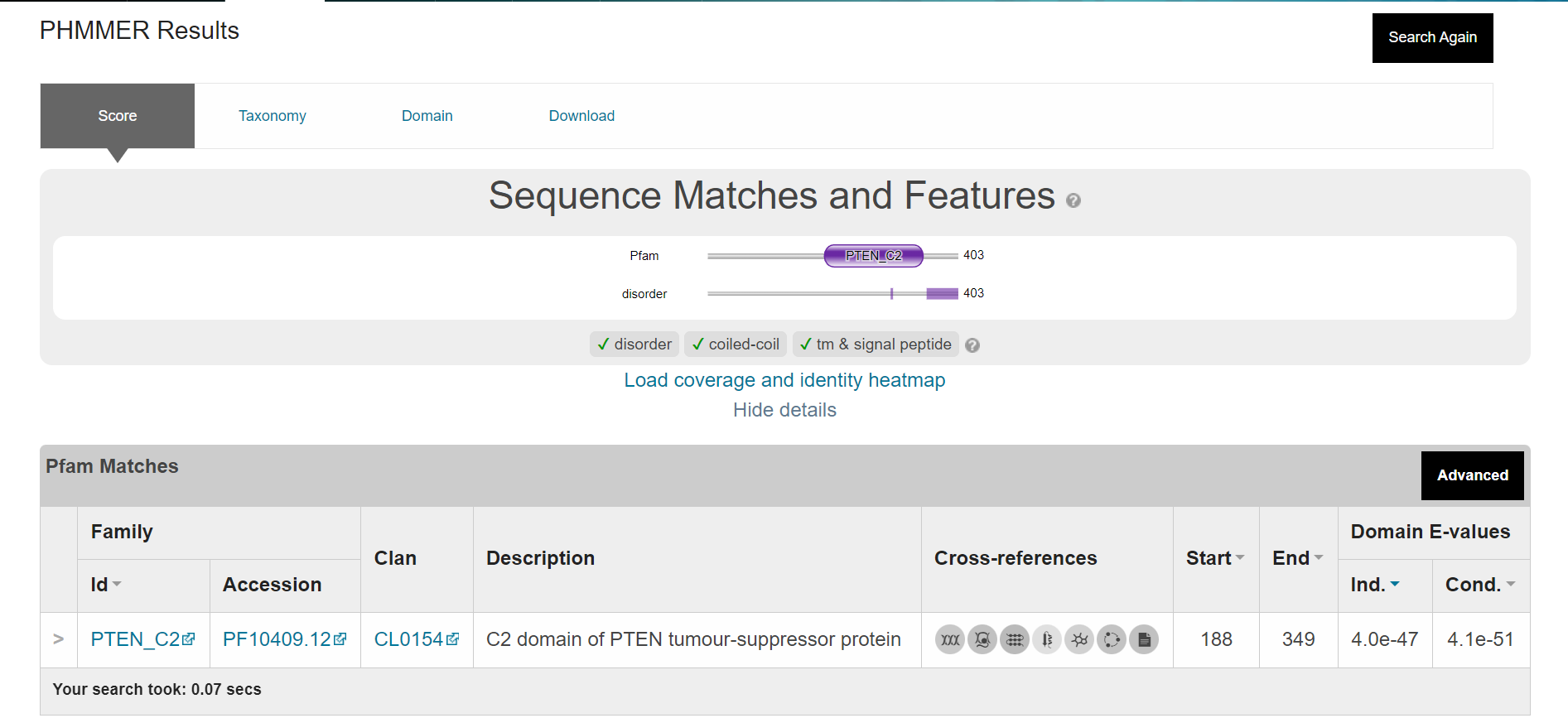
Protein Name: phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN isoform PTEN [Homo sapiens]

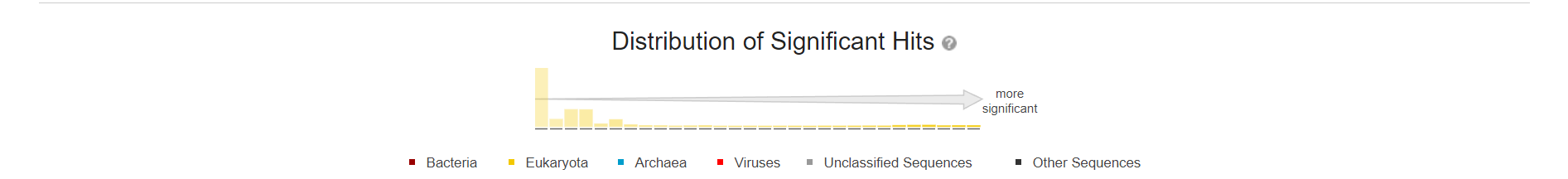
Protein ID: P60484 (UniProt)

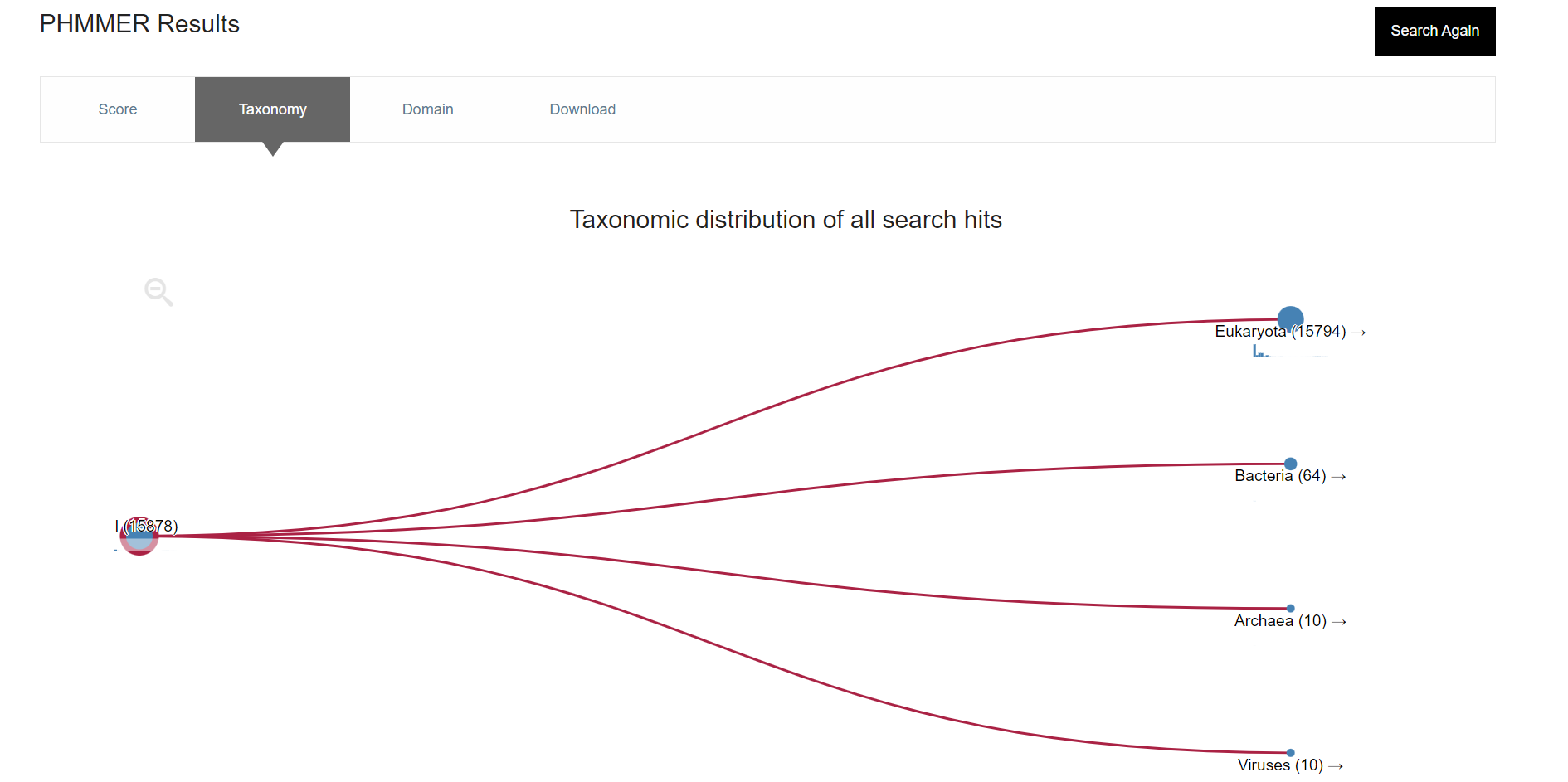
Accession no. – NP\_000305

Motif: PDZ domain binding motif (401-403)

**HMMER:**



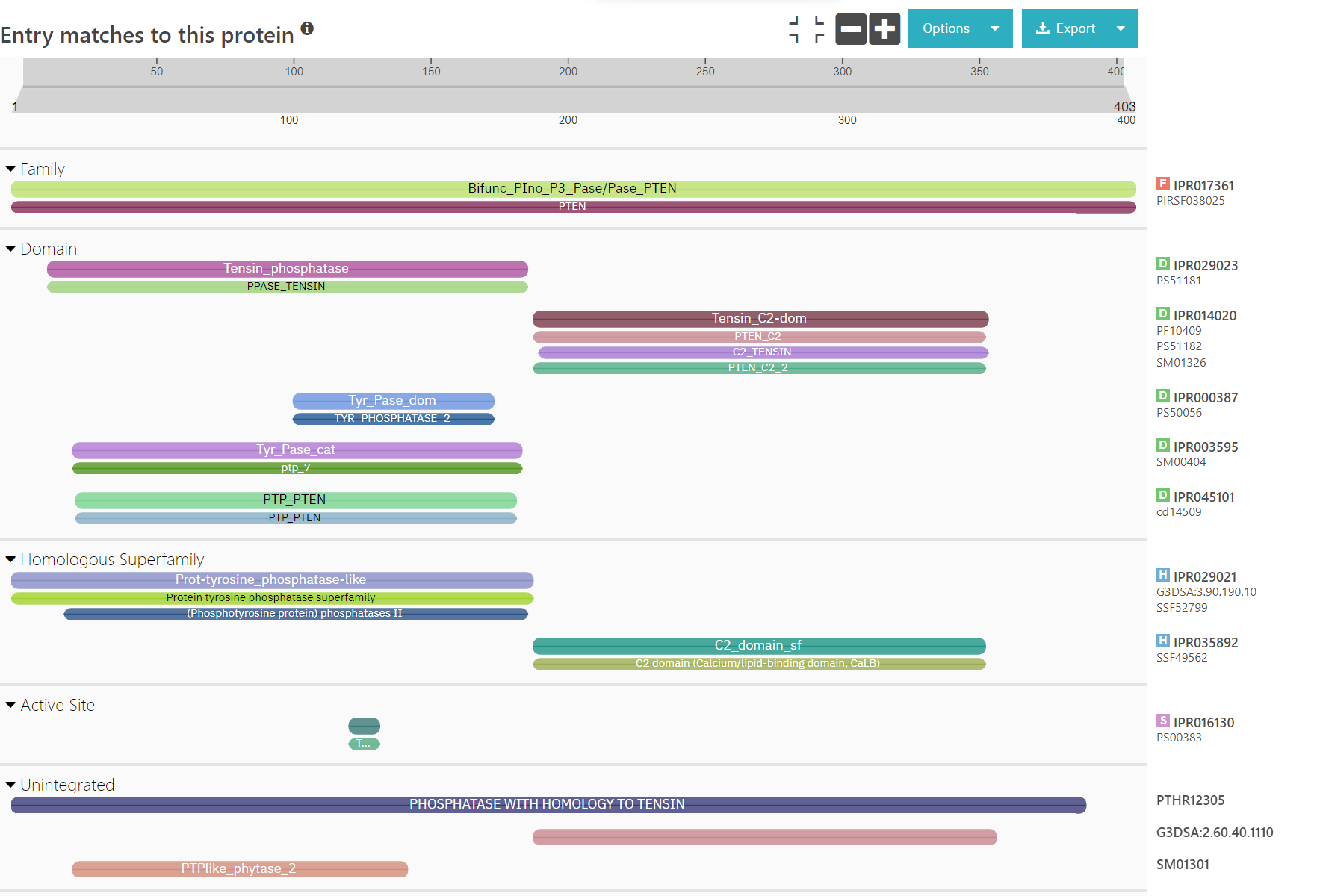
****



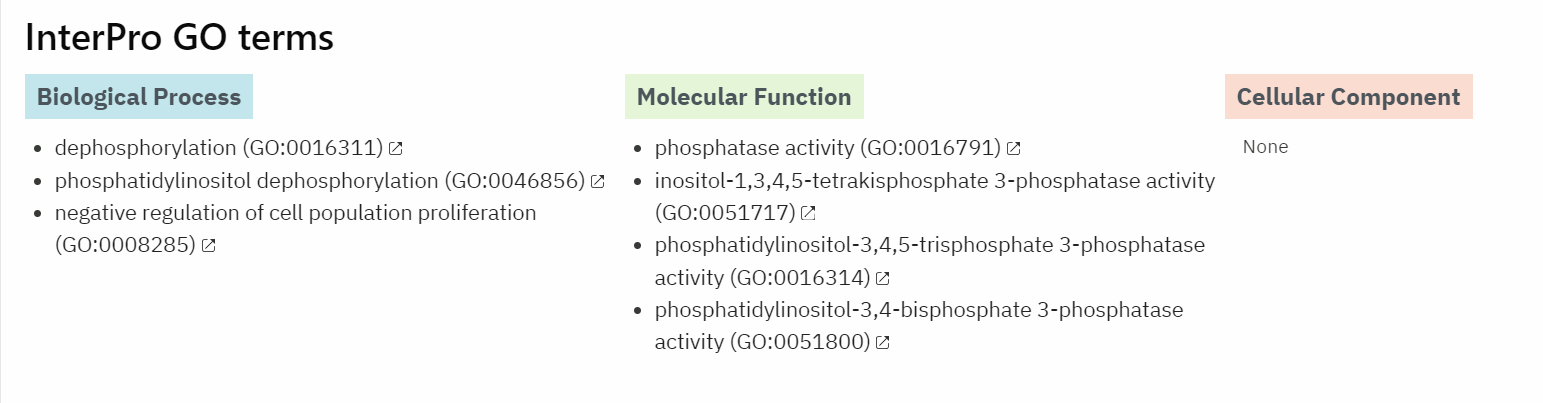
**InterProScan:**

**Family –** Bifunctional phosphatidylinositol trisphosphate phosphatase/dual specificity phosphatase PTEN

**Domains –** Tensin-type phosphatase domain; Tensin phosphatase, C2 domain; Tyrosine-specific protein phosphatases domain; Protein-tyrosine phosphatase, catalytic domain; PTEN, phosphatase domain

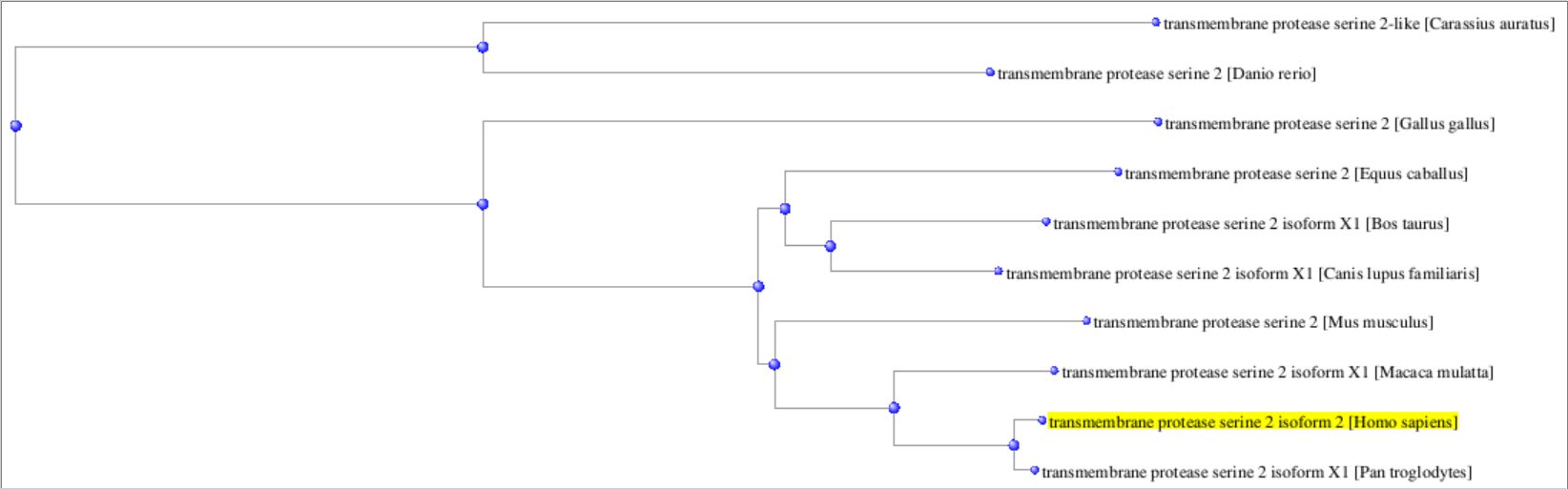


**Functions:**

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**Day 3: Phylogenetics**

**Constructing a Phylogenetic tree for component of Corona virus.**

****

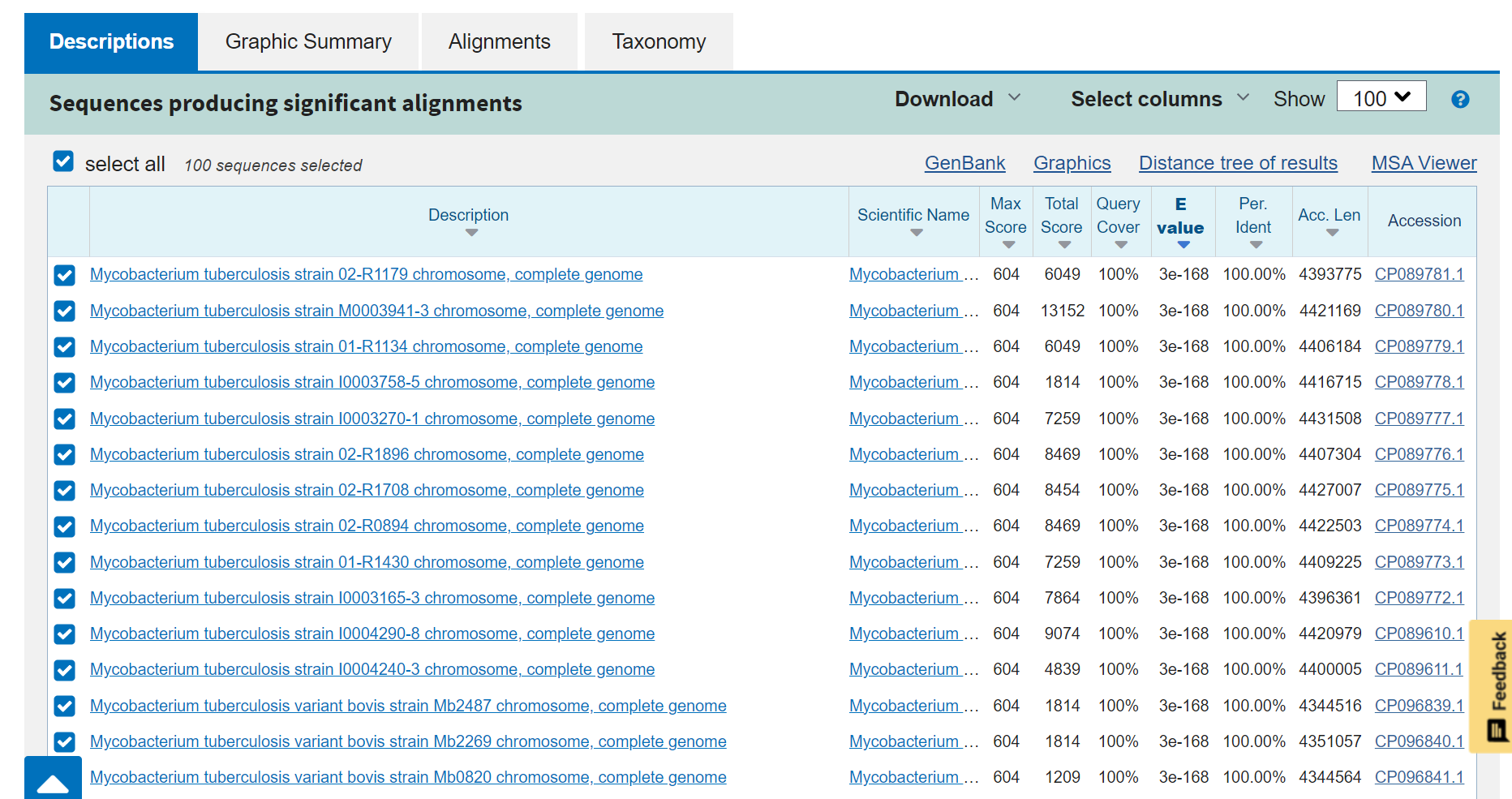
**Day 4:**

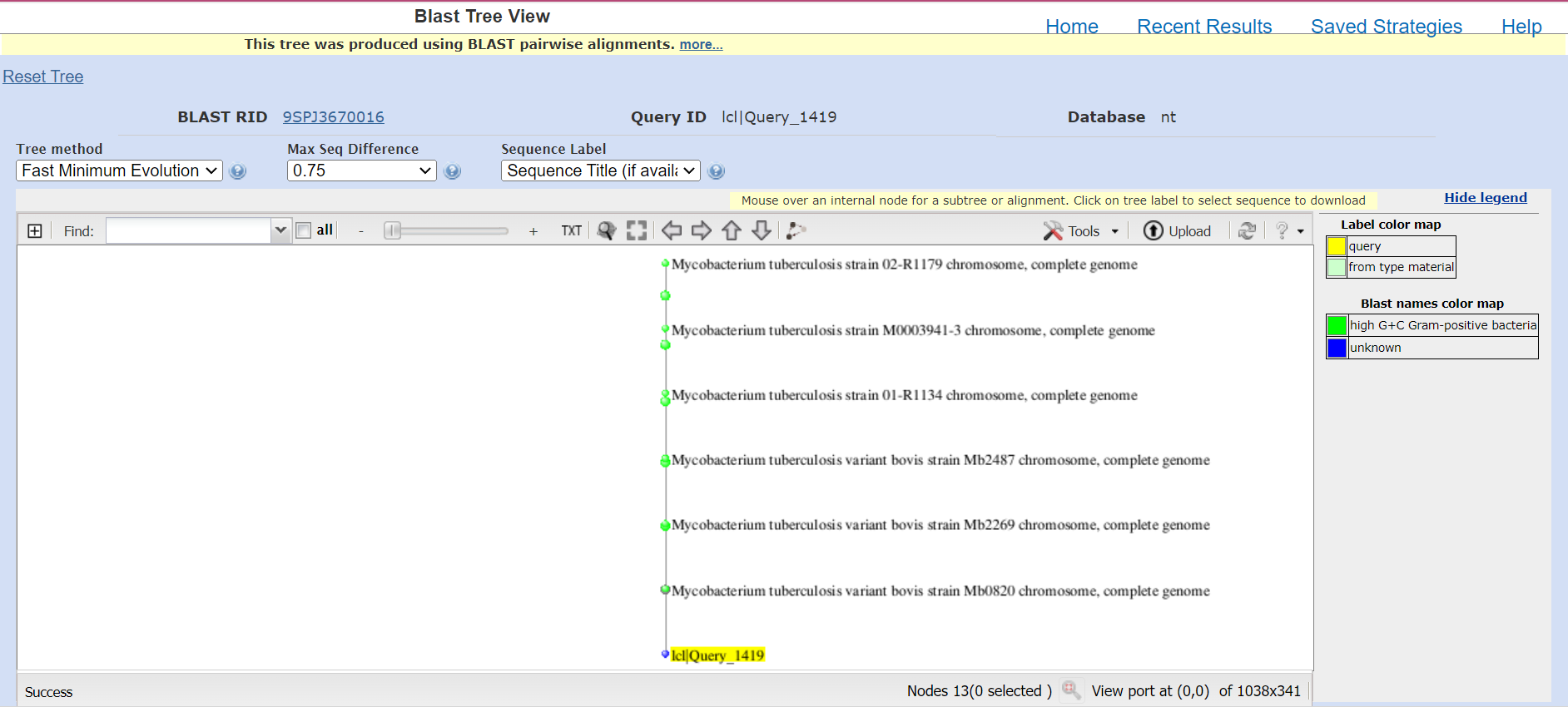
**Genome name: Mycobacterium tuberculosis**

**From RAST results:**

1. Nucleotide sequence - atgtcaggtggttcatcgaggaggtacccgccggagctgcgtgagcgggcggtgcggatggtcgcagagatccgcggtcagcacgattcggagtgggcagcgatcagtgaggtcgcccgtctacttggtgttggctgcgcggagacggtgcgtaagtgggtgcgccaggcgcaggtcgatgccggcgcacggcccgggaccacgaccgaagaatccgctgagctgaagcgcttgcggcgggacaacgccgaattgcgaagggcgaacgcgattttaaagaccgcgtcggctttcttcgcggccgagctcgaccggccagcacgctaa
2. Location on the genome - AL123456.3\_889072\_889398
3. Start nucleotide – 889072
4. End nucleotide – 889398
5. Function - Insertion element IS6110 (Mycobacterium tuberculosis) transposase

**Perform a BLAST on the nucleotide sequence and paste a screenshot of the obtained BLAST results:**





**Day 5 & 6:**

**Molecular Docking**

Protein Name: TLR1-TLR2 heterodimer induced by binding of a tri-acylated lipopeptide

Protein ID – 2Z80

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Ligand Name | Ligand ID | Follows Lipinski Rule? | Energy value | Dock Image |
| Isoniazid | 3767 | Yes | 96.25 |  |
| Pyrazinamide | 1046 | Yes | 61.32 |  |
| Ethambutol | 14052 | Yes | 159.47 |  |

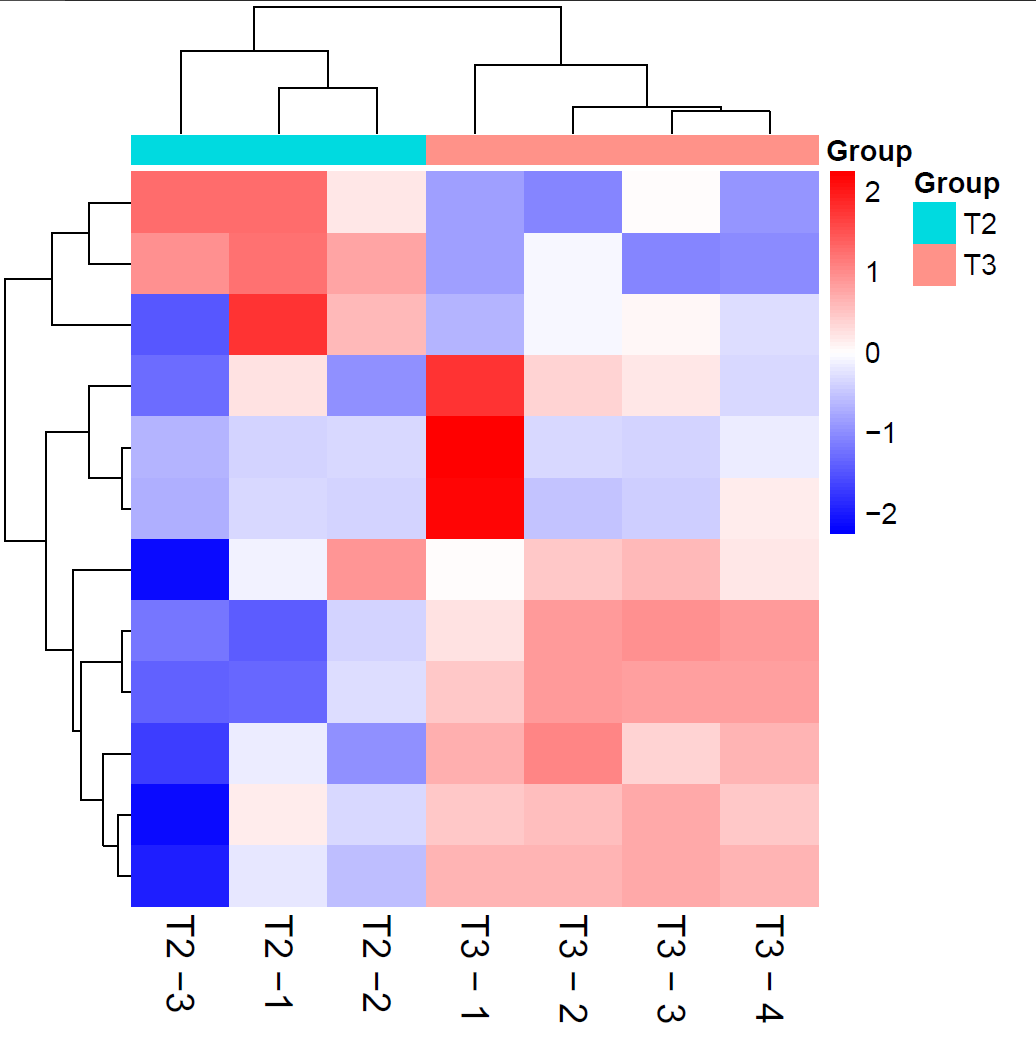
**Day 7:**

**Reference:** Vivek K. Mutalik, Benjamin A. Adler, Harneet S. Rishi, Denish Piya, Crystal Zhong, Britt Koskella, Elizabeth M. Kutter, Richard Calendar, Pavel S. Novichkov, Morgan N. Price, Adam M. Deutschbauer, Adam P. Arkin.High-throughput mapping of the phage resistance landscape in E. coli. doi: <https://doi.org/10.1371/journal.pbio.3000877> -

**Table:** E. coli K-12 RB-TnSeq data for 2 dsDNA phages at different MOI

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Group** | **T2** | **T2** | **T2** | **T3** | **T3** | **T3** | **T3** |
| **Phage** | **T2 -1** | **T2 -2** | **T2 -3** | **T3 - 1** | **T3 - 2** | **T3 - 3** | **T3 - 4** |
| cyaA | 3.58 | 3.12 | 1.46 | 3.89 | 3.96 | 4.14 | 3.89 |
| dgcJ | 1.13 | 0.91 | 0.85 | 1.41 | 1.16 | 1.12 | 1.02 |
| dnaJ | 0.78 | 1.17 | 0.04 | 0.83 | 1.01 | 1.05 | 0.91 |
| envZ | 1.03 | 0.91 | 0.15 | 7.13 | 0.59 | 0.80 | 2.19 |
| fadL | 16.75 | 13.88 | 15.11 | 2.60 | 7.90 | 1.10 | 1.33 |
| fhuA | -0.19 | -0.08 | -0.93 | 6.45 | -0.05 | -0.18 | 0.39 |
| galU | 3.65 | 3.28 | 2.61 | 2.87 | 3.05 | 3.10 | 2.99 |
| igaA | 6.30 | 10.46 | 7.26 | 12.96 | 15.52 | 15.80 | 15.56 |
| lamB | 0.23 | 0.04 | -0.14 | 0.44 | 0.53 | 0.36 | 0.43 |

**Heatmap:**

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**Day 8 & 9: Homology Modelling:**

**Problem statement:** To visualize the 3D structure of **Neuropilin-1** by homology modelling

**Protein:** **Neuropilin-1**

**Gene:** **NRP1**

**PDB:** O14786 (First Isoform)

**Hypothesis:** Homology modelling of Neuropilin-1 will provide insights into its interaction with the SARS-CoV-2 spike protein and the CendR motif RRAR, enabling a better understanding of the mechanism by which Neuropilin-1 enhances SARS-CoV-2 infection.

**Purpose:** The purpose of this study is to develop a 3D structure of Neuropilin-1 using homology modelling to elucidate the molecular details of its interaction with the SARS-CoV-2 spike protein. By gaining a structural understanding of this interaction, we aim to investigate the role of Neuropilin-1 as a host factor for SARS-CoV-2 infection and the specific binding mechanism involving the CendR motif RRAR.

**Outcome:** The outcome of this study will be a reliable 3D model of Neuropilin-1, which can be used to identify key residues involved in the recognition and binding of the CendR motif RRAR on the SARS-CoV-2 spike protein S1. This structural information can potentially aid in the development of therapeutics that target the interaction between Neuropilin-1 and SARS-CoV-2, aiming to disrupt or inhibit this interaction and reduce the infectivity of the virus. Additionally, understanding the structural basis of the Neuropilin-1/SARS-CoV-2 interaction may also provide insights into the general mechanisms of viral infection and host factors involved in viral entry, potentially leading to the development of broader antiviral strategies.

|  |  |  |
| --- | --- | --- |
| **Target** | **Sequence** | **Result** |
|  |  |  |

**Day 10:**

Please paste your GitHub account link: [github.com/Arun0364](https://github.com/Arun0364)