BV-BRC Test Report

A15. Service – MSA and SNP

| Item to test | MSA and SNP Service using bacterial and viral gene and protein sequences |
|---------------|---|
| URL | https://www.bv-brc.org/app/MSA |
| Prerequisites | Bacterial and viral feature groups and FASTA sequence files |
| References | https://www.bv-brc.org/docs/quick references/services/msa snp variation service.html https://www.bv-brc.org/docs/tutorial/msa snp variation/msa snp variation.html |
| Tester(s) | Christian Zmasek, Yun Zhang, Maulik Shukla |
| Test date | 08-May-2022 (follow-up from original test) |
| Test result | Passed |

Overview

- Test the MSA and SNP Service using exemplar bacterial and viral gene and protein sequences.
- Test input options, i.e., feature groups, fasta sequence files, and sequence input box.
- Test different MSA algorithms, MAFFT and Muscle.
- For each job submitted, verify successful completion of the job, presence of output files in various formats, review resulting MSA and SNPs.
- View MSA using interactive MSA viewer and verify all functionality.

Test Data

| Dataset | Rational | Input Format | Input | | | | |
|-------------------------|-----------------------------------|------------------------------|----------------------------------|--|--|--|--|
| SARSCoV2 spike proteins | Viral proteins of interest | Feature group, FASTA file | SARSCoV2_Spike_protein.f asta | | | | |
| MTB ahpD proteins | Bacterial proteins of interest | Feature group, FASTA file | MTB_ahpD_protein.fasta | | | | |

 All test datasets and corresponding job results are available in the following public workspace: <u>https://www.bv-</u> brc.org/workspace/BVBRC@patricbrc.org/BVBRC%20Tests/Multiple%20Sequence%20Alignment

Test Results

- All MSA jobs completed successfully, without any errors.
- All jobs resulted in expected output files in corresponding job output directory, including alignment in afa, nexus, phy, and pir formars and consensus sequence in fasta format.
- SNPs were present as a tsv file in the expected format and the tsv viewer allow filtering and sorting of the table based on the SNP scores.

- The link to MSA viewer loaded the MSA and all functionality worked as expected, including changing node labels, and showing / hiding positions based on conservation.
- All test datasets and corresponding job results are available in the following public workspace: <u>https://www.bv-</u>

brc.org/workspace/BVBRC@patricbrc.org/BVBRC%20Tests/Multiple%20Sequence%20Alignment

• Below are a series of screenshots showing successful completion of the jobs, availability of the result files in the workspace, and the MSA viewer.

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| completed | 7747116 | MSA | SARSCov2 Spike Protein - Nonhuman Mammals - MSA | 5/7/22, 5:05 PM | 5/7/22, 5:05 PM | 5/7/22, 5:06 PM |
| completed | 7747808 | MSA | MTB ahpD protein - MSA | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM |
| completed | 7747809 | MSA | MTB ahpD protein - NA | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM |
| completed | 7747810 | MSA | MTB ahpD protein - AA | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM | 5/8/22, 4:28 PM |
| completed | 7747811 | MSA | MTB ahpD protein - AA - Muscle | 5/8/22, 4:29 PM | 5/8/22, 4:29 PM | 5/8/22, 4:29 PM |
| completed | 7747812 | MSA | SARSCoV2 Spike protein - MSA | 5/8/22, 4:29 PM | 5/8/22, 4:29 PM | 5/8/22, 4:29 PM |
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| completed | 7747815 | MSA | SARSCoV2 Spike protein - AA | 5/8/22, 4:30 PM | 5/8/22, 4:30 PM | 5/8/22, 4:30 PM |
| completed | 7747816 | MSA | SARSCoV2 Spike protein - AA | 5/8/22, 4:30 PM | 5/8/22, 4:30 PM | 5/8/22, 4:30 PM |
| completed | 7747817 | MSA | SARSCoV2 Spike protein - AA - Muscle | 5/8/22, 4:30 PM | 5/8/22, 4:30 PM | 5/8/22, 4:31 PM |
| completed | 7747827 | MSA | MTB ahpD protein - AA - fasta | 5/8/22, 5:00 PM | 5/8/22, 5:00 PM | 5/8/22, 5:01 PM |
| completed | 7747831 | MSA | SARSCoV2 Spike protein - fasta | 5/8/22, 5:01 PM | 5/8/22, 5:01 PM | 5/8/22, 5:01 PM |
| completed | 7747832 | MSA | SARSCoV2 Spike protein - seq | 5/8/22, 5:04 PM | 5/8/22, 5:04 PM | 5/8/22, 5:04 PM |

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| 89 | SARSCoV2 Spike protein - seq input | 39.3 kB | me | Public | 5/8/22, 5:04 PM | |
| 6 3 | SARSCoV2 Spike protein - fasta | 7.1 kB | me | Public | 5/8/22, 5:01 PM | |
| 83 | SARSCoV2 Spike protein - NA | 6.9 kB | me | Public | 5/8/22, 4:31 PM | |
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| 83 | SARSCoV2 Spike protein - MSA | 6.9 kB | me | Public | 5/8/22, 4:29 PM | |
| 83 | SARSCoV2 Spike protein - AA - Muscle | 7.1 kB | me | Public | 5/8/22, 4:31 PM | |
| 83 | SARSCoV2 Spike protein - AA | 7.1 kB | me | Public | 5/8/22, 4:30 PM | |
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| | MTB_ahpD_protein.fasta | 15.6 kB | me | Public | 5/8/22, 4:59 PM | |
| 83 | MTB ahpD protein - NA | 6.8 kB | me | Public | 5/8/22, 4:28 PM | |
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| 89 | MTB ahpD protein - AA - fasta | 7.0 kB | me | Public | 5/8/22, 5:00 PM | |
| 83 | MTB ahpD protein - AA - Muscle | 7.0 kB | me | Public | 5/8/22, 4:29 PM | |
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| | 452 | 94 | Leu | Arg=4,GIn=1,Leu=17 | 22 | | |
| | 501 | 85 | Asn | Asn=16,Tyr=6 | 22 | | |
| | 152 | 79 | Trp | Arg=1,Cys=1,Leu=1,Trp=19 | 22 | | |
| | 69 | 77 | His | Del=5,His=17 | 22 | | |
| | 70 | 77 | Val | Del=5,Val=17 | 22 | | |
| | 417 | 70 | Lys | Asn=2,Lys=19,Thr=1 | 22 | | |
| | 95 | 68 | Thr | Ile=4,Thr=18 | 22 | | |
| | 1027 | 68 | Thr | Ile=4,Thr=18 | 22 | | |
| | 242 | 57 | Leu | Del=3,Leu=19 | 22 | | |
| | 243 | 57 | Ala | Ala=19,Del=3 | 22 | | |
| | 655 | 57 | His | His=19,Tyr=3 | 22 | | |
| | 716 | 57 | Thr | Ile=3,Thr=19 | 22 | | |
| | 145 | 53 | Tyr | Del=1,Ser=1,Tyr=20 | 22 | | |
| | 156 | 53 | Glu | Del=1,Glu=20,Gly=1 | 22 | | |
| | 253 | 53 | Asp | Asn=1,Asp=20,Gly=1 | 22 | | |
| | 346 | 53 Arg Arg=20,Lys=1,Ser=1 | | | | | |
| | 796 | 53 | Asp | Asp=20,His=1,Tyr=1 | 22 | | |
| | 5 | 44 | Leu | Leu=20,Phe=2 | 22 | | |
| | 18 | 44 | Leu | Leu=20,Phe=2 | 22 | | |
| | 26 | 44 | Pro | Pro=20,Ser=2 | 22 | | |
| | 67 | 44 | Ala | Ala=20,Val=2 | 22 | | |
| | 142 | 44 | Gly | Asp=2,Gly=20 | 22 | | |
| | 157 | 44 | Phe | Del=2,Phe=20 | 22 | | |
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| Image Image </td <td>$\begin{array}{c} L \ P \ S \ S \ L \\ L \ P \ S \ S \ L \ L \ P \ S \ S \ L \\ L \ P \ S \ S \ L \ L \ S \ S \ L \ L \ P \ S \ S \ S \ L \ L \ S \ S \ S \ S \ S$</td> <td></td> <td>A H V G A - - G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H</td> <td>T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V</td> <td>$\begin{array}{c} {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf Y} \ {\bf V} \\ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \\ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf C} \ {\bf C} \ {\bf D} \ {\bf C}$</td> <td>Y K K K K K K K K K K K</td> <td></td> <td>$\begin{array}{cccccccccccccccccccccccccccccccccccc$</td> <td>- D L L A - D L L A - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L</td> <td>H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I</td> <td>$\begin{array}{c} T \ P \ G \ L \\ T \ P \ G \ L \ T \ P \ G \ L \\ T \ P \ G \ L \ T \ P \ C \ T \ P \ C \ L \ T \ P \ C \ L \ T \ P \ C \ L \ T \ P \ C \ T \ P \ C \ T \ T \ P \ C \ T \ T \ T \ T \ T \ T \ T \ T \ T$</td> <td>> F G R N > F G R N</td> <td>S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S L P F S S S S S S</td> <td>2 K K N K V C 2 K N K V C 2 K N N V C 2 K N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N V C 2 Z X X X X X X X X X X X X X X X X X X</td> <td>G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y</td> | $ \begin{array}{c} L \ P \ S \ S \ L \\ L \ P \ S \ S \ L \ L \ P \ S \ S \ L \\ L \ P \ S \ S \ L \ L \ S \ S \ L \ L \ P \ S \ S \ S \ L \ L \ S \ S \ S \ S \ S$ | | A H V G A - - G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H V G A H | T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V T D T V | $ \begin{array}{c} {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf Y} \ {\bf V} \\ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \\ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf G} \ {\bf V} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf V} \ {\bf C} \ {\bf D} \ {\bf C} \ {\bf C} \ {\bf C} \ {\bf D} \ {\bf C} $ | Y K K K K K K K K K K K | | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | - D L L A - D L L A - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L - D L L L | H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I H R S Y I | $\begin{array}{c} T \ P \ G \ L \\ T \ P \ G \ L \ T \ P \ G \ L \\ T \ P \ G \ L \ T \ P \ C \ T \ P \ C \ L \ T \ P \ C \ L \ T \ P \ C \ L \ T \ P \ C \ T \ P \ C \ T \ T \ P \ C \ T \ T \ T \ T \ T \ T \ T \ T \ T$ | > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N > F G R N | S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S S L P F S S S S S S | 2 K K N K V C 2 K N K V C 2 K N N V C 2 K N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N N V C 2 Z X X N V C 2 Z X X X X X X X X X X X X X X X X X X | G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y N L S T G Y |

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