IgFamily v0.9.9

Technical manual v0.1

Features

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**- FASTA utility tools:**

Read FASTA files into runtime. Custom FASTA creation utility provides functionality for tailored output files. This utlility can be used to create required FASTA format –

>[ACCESSION]|[NAME]|[TYPE]|[SPECIES]|

Accession field is a housekeeping field and is not required for runtime. Name, type, and species fields are used in data structure creation, association, and function.

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| FASTA parse function | pp. |
| FASTA file utilities | pp. |

**- Peptide file parsing:**

Read peptide files into runtime. Currently supported are *PEAKS v8.0 DE NOVO* de novo peptides .csv export, *PEAKS v8.0 SPIDER* protein peptide .csv export, and *NOVOR v1.1* de novo peptides .csv export.

*PEAKS v8.0 DE NOVO* de novo peptides peptide file assigns peptide with modification and amino acid local confidence score. Note that here *PEAKS* *v8.0 DE NOVO* assigns individual export accesions to replicate peptide assignments.

*PEAKS v8.0 SPIDER* protein peptide file assigns peptide with modification, spectral count, and -10IgP certainty score.

*NOVOR v1.1* de novo peptides file assigns peptide with modification and amino acid local confidence score. Note that here *NOVOR v1.1* assigns individual export accesions to replicate peptide assignments.

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| Peptide file parse functions | pp. |

**- *msconvert* external integration**

*msconvert* is able to be called through a user defined interface option to convert .wiff and .wiff.scan files into the *Mascot Generic Format* .mgf file type. Various command line options may be selected with peak-picking as the default option. The generated file is created in the same folder as the input file.

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| *msconvert* convert command line functions | pp. |
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**- *NOVOR v1.1* external integration**

*NOVOR v1.1* is able to be called through a user defined interface option to generate *NOVOR v1.1* de novo peptide files in the .csv file type. Various command line options may be selected. The generated file is created in the same folder as the input file.

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| *NOVOR v1.1* convert command line functions | pp. |

**- Local directory runtime functionality**

The *IgFamily* program is able to be run in local directory or filesystem directory file mode. In local directory file mode the user places the required files in the *IgFamily* root directory and executes the program. The input file and output files are moved to a folder created in the root directory with the name of the input file sample - The input file contains the sample name and is supported in the three input data types.

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| Local directory runtimefunctions | pp. |

**- Data filesystem**

The *IgFamily* program is able to be run in local directory or filesystem directory file mode. In filesystem mode the program accessions a dedicated file association structure to retrieve and export files. The filesystem is currently defined on the *FATELVIS* network assisted storage device. The user is required to accession a file initially, however there is proposed functionality for dynamic file management with the *ISO/IEC TS 18822:2015* filesystem library.

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| Data filesystem functions | pp. |

**- Runtime user interface**

On execution of the *IgFamily* program, the user is greeted with an interactive menu. The user is able to access FASTA file utilities, *msconvert* command line tools, *NOVOR v1.1* command line tools, and select program parameters. Program parameters include local or filesystem file modes, FASTA file selection, and peptide assignment selection.

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| User interface functions | pp. |

Production

Version: v0.9.6

Release: 2016-09-17

Codebase: 4,857 source lines of code

Dependency: 18 files

Version history: 139 commits

Codebase additions: 21,040 source lines of code

Codebase deletions: 16,083 source lines of code

Development environment: Microsoft Visual Studio Community 2015

Version control: Git