NAME

InfoNucleicAcids.pl - List properties of nucleic acids

SYNOPSIS

InfoNucleicAcids.pl NucleicAcidIDs...

InfoNucleicAcids.pl [-h, --help] [-m, --mode NucleicAcidID | NucleicAcidType] [--OutDelim comma | tab | semicolon] [--output STDOUT | File] [--OutputStyle NucleicAcidBlock | NucleicAcidRows] [-o, --overwrite] [--precision number] [--PropertiesMode Categories | Names | All] [-p, --properties CategoryName, [CategoryName,...] | PropertyName, [PropertyName,...]] [--PropertiesListing ByGroup | Alphabetical] [-q, --quote yes | no] [-r, --root rootname] [-w, --WorkingDir dirname] NucleicAcidIDs...

DESCRIPTION

List nucleic acid properties. Nucleic acids identification supports two types of IDs: code or name. Nucleic acid properties data, in addition to basic information about nucleic acids - code, name, type, chemical formula and molecular weight - include information about exact mass and elemental composition.

PARAMETERS

NucleicAcidI Ds Code [NucleicAcidName...] | NucleicAcidType [NucleicAcidType...]

NucleicAcidIDs is a space delimited list of values to identify nucleic acids.

For NucleicAcidID mode, input value format is: Code [NucleicAcidName...]. Default: A. Examples:

```
A dG AMP Cytidine T UDP dpppA "5'-dATP"
```

For NucleicAcidType mode, input value format is: NucleicAcidType [NucleicAcidType...]. Default: A. Possible values are: Nucleoside, Nucleoside, Deoxynucleoside, Nucleoside. Default: Nucleoside. Examples:

Deoxynucleoside Nucleobase Nucleotide

OPTIONS

-h, --help

Print this help message.

-m, --mode NucleicAcidID | NucleicAcidType

Specify nucleic acids for listing properties using one of these methods: nucleic acid code and/or names or nucleic acid type.

Possible values: NucleicAcidID or NucleicAcidType. Default: NucleicAcidID

For NucleicAcidType, command line parameters support these type: Nucleobase, Nucleoside, Deoxynucleoside, Nucleotide, Deoxynucleotide.

--OutDelim comma | tab | semicolon

Output text file delimiter. Possible values: comma, tab, or semicolon Default value: comma.

--output STDOUT | File

List information at STDOUT or write it to a file. Possible values: *STDOUT or File*. Default: *STDOUT*. -r, --root option is used to generate output file name.

-- OutputStyle NucleicAcidBlock | NucleicAcidRows

Specify how to list nucleic acid information: add a new line for each property and present it as a block for each nucleic acid; or include all properties in one line and show it as a single line.

Possible values: NucleicAcidBlock | NucleicAcidRows. Default: NucleicAcidBlock

An example for NucleicAcidBlock output style:

Code: Ado
OtherCodes: A
Name: Adenosine
Type: Nucleoside

MolecularFormula: C10H13O4N5 MolecularWeight: 267.2413

.

An example for NucleicAcidRows output style:

Code, OtherCodes, Name, Type, MolecularFormula, MolecularWeight

-o, --overwrite

Overwrite existing files.

--precision number

Precision for listing numerical values. Default: up to 4 decimal places. Valid values: positive integers.

-- Properties Mode Categories | Names | All

Specify how property names are specified: use category names; explicit list of property names; or use all available properties. Possible values: *Categories, Names, or All.* Default: *Categories*.

This option is used in conjunction with -p, --properties option to specify properties of interest.

-p, --properties CategoryName,[CategoryName,...] | PropertyName,[PropertyName,...]

This option is --propertiesmode specific. In general, it's a list of comma separated category or property names.

Specify which nucleic acid properties information to list for the nucleic acid IDs specified using command line parameters: list basic information; list all available information; or specify a comma separated list of nucleic acid property names.

Possible values: Basic | BasicPlus | PropertyName,[PropertyName,...]. Default: Basic.

Basic includes: Code, OtherCodes, Name, Type, MolecularFormula, MolecularWeight

BasicPlus includes: Code, OtherCodes, Name, Type, MolecularFormula, MolecularWeight, ExactMass, ElementalComposition

Here is a complete list of available properties: Code, OtherCodes, BasePair, Name, Type, MolecularFormula, MolecularFormulaAtpH7.5, MolecularWeight, ExactMass, ElementalComposition.

-- PropertiesListing ByGroup | Alphabetical

Specify how to list properties for nucleic acids: group by category or an alphabetical by property names. Possible values: *ByGroup or Alphabetical*. Default: *ByGroup*

-q, --quote yes | no

Put quotes around column values in output text file. Possible values: yes or no. Default value: yes.

-r, --root rootname

New text file name is generated using the root: <Root>.<Ext>. File name is only used during *File* value of -o, --output option.

Default file name: NucleicAcidInfo<mode>.<Ext>. The csv, and tsv <Ext> values are used for comma/semicolon, and tab delimited text files respectively.

-w, --WorkingDir dirname

Location of working directory. Default: current directory.

EXAMPLES

To list basic properties information for nucleoside A, type:

% InfoNucleicAcids.pl

To list all available properties information for nucleoside A, type:

% InfoNucleicAcids.pl --propertiesmode all A

To list all available information for all available nucleic acids, type:

% InfoNucleicAcids.pl --propertiesmode All All

To list basic properties information for all nucleobases, type:

% InfoNucleicAcids.pl -m NucleicAcidType Nucleoside

To list basic properties information for all nucleotides and deoxynulceotides, type:

% InfoNucleicAcids.pl -m NucleicAcidType Nucleotide Deoxynucleotide

To list basic properties information for variety of nucleic acids, type:

% InfoNucleicAcids.pl A dG AMP Cytidine T UDP "5'-dATP"

To list code and molecular weights for nucleosides A, G, C and T, type:

% InfoNucleicAcids.pl --PropertiesMode Names --properties
Code,MolecularWeight A G C T

To alphabetically list all the available properties for nucleotides dAMP, dGMP, dCMP, and dTMP in rows instead of nucleic acid blocks with quotes around the values, type:

% InfoNucleicAcids.pl --PropertiesMode All --PropertiesListing
Alphabetical --OutputStyle NucleicAcidRows -q yes dAMP dGMP
dCMP dTMP

To alphabetically list all the available properties for all available nucleic acids to a file names NucleicAcidsProperties.csv with quotes around the values, type

% InfoNucleicAcids.pl --PropertiesMode All --PropertiesListing Alphabetical --output File --OutputStyle NucleicAcidRows -r NucleicAcidsProperties -o -q Yes All

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

InfoAminoAcids.pl, InfoPeriodicTableElements.pl

COPYRIGHT

Copyright (C) 2017 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.