NAME

InfoAminoAcids.pl - List properties of amino acids

SYNOPSIS

InfoAminoAcids.pl AminoAcidIDs...

```
InfoAminoAcids.pl [-h, --help] [--outdelim comma | tab | semicolon] [--output STDOUT | File] [ --outputstyle AminoAcidBlock | AminoAcidRows] [-o, --overwrite] [--precision number] [ --propertiesmode Categories | Names | All] [-p, --properties CategoryName, [CategoryName,...] | PropertyName, [PropertyName,...] [--propertieslinting ByGroup | Alphabetical] [-q, --quote yes | no] [-r, --root rootname] [-w, --workingdir dirname] AminoAcidIDs...
```

DESCRIPTION

List amino acid properties. Amino acids identification supports these three types of IDs: one letter code, three letter code or name. Amino acid properties data, in addition to basic information about amino acids - one and three letter codes, name, DNA and RNA codons, molecular weight - include variety of other properties: polarity, acidity, hydrophobicity, and so on.

PARAMETERS

AminoAcidI Ds ThreeLetterCode [OneLetterCode AminoAcidName...]

AminoAcidIDs is a space delimited list of values to identify amino acids.

Input value format is: ThreeLetterCode [OneLetterCode AminoAcidName...]. Default: Ala. Examples:

```
Ala
Glu A
Alanine Glu Y "Aspartic acid"
```

OPTIONS

```
-h, --help
```

Print this help message.

--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 AminoAcidBlock | AminoAcidRows

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

Possible values: AminoAcidBlock | AminoAcidRows. Default: AminoAcidBlock

An example for AminoAcidBlock output style:

```
ThreeLetterCode: Ala
OneLetterCode: A
AminoAcid: Alanine
MolecularWeight: 89.0941
.....
ThreeLetterCode: Glu
OneLetterCode: E
AminoAcid: Glutamic acid
MolecularWeight: 147.1308
.....
```

An example for $\it AminoAcidRows$ output style:

```
ThreeLetterCode,OneLetterCode,AminoAcid,MolecularWeight Ala,A,Alanine,89.0941..
Glu,E,Glutamic acid,147.1308..
```

-o, --overwrite

Overwrite existing files.

--precision number

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

--propertiesmode 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 amino acid properties information to list for the amino acid IDs specified using command: line parameters: list basic and/or hydrophobicity information; list all available information; or specify a comma separated list of amino acid property names.

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

Basic includes: ThreeLetterCode, OneLetterCode, AminoAcid, DNACodons, RNACodons, ChemicalFormula, MolecularWeight, LinearStructure, LinearStructureAtpH7.4

BasicPlus includes: ThreeLetterCode, OneLetterCode, AminoAcid, DNACodons, RNACodons, AcidicBasic, PolarNonpolar, Charged, Aromatic, HydrophobicHydophilic, IsoelectricPoint, pKCOOH, pKNH3+, ChemicalFormula, MolecularWeight, ExactMass, ChemicalFormulaMinusH2O, MolecularWeightMinusH2O(18.01524), ExactMassMinusH2O(18.01056), LinearStructure, LinearStructureAtpH7.4

BasicAndHydrophobicity includes: ThreeLetterCode, OneLetterCode, AminoAcid, DNACodons, RNACodons, ChemicalFormula, MolecularWeight, LinearStructure, LinearStructureAtpH7.4, HydrophobicityEisenbergAndOthers, HydrophobicityHoppAndWoods, HydrophobicityJanin, HydrophobicityKyteAndDoolittle, HydrophobicityRoseAndOthers, HydrophobicityWolfendenAndOthers

BasicAndHydrophobicityPlus includes: (ThreeLetterCode, OneLetterCode, AminoAcid, DNACodons, RNACodons, ChemicalFormula, MolecularWeight, LinearStructure, LinearStructureAtpH7.4, HydrophobicityAbrahamAndLeo, HydrophobicityBlack, HydrophobicityBullAndBreese, HydrophobicityChothia, HydrophobicityEisenbergAndOthers, HydrophobicityFauchereAndOthers, HydrophobicityGuy, HydrophobicityHPLCAtpH3.4Cowan, HydrophobicityHPLCAtpH7.5Cowan, HydrophobicityHPLCParkerAndOthers, HydrophobicityHPLCWilsonAndOthers, HydrophobicityHoppAndWoods, HydrophobicityJanin, HydrophobicityKyteAndDoolittle, HydrophobicityManavalanAndOthers, HydrophobicityMiyazawaAndOthers, HydrophobicityOMHSweetAndOthers, HydrophobicityRaoAndArgos, HydrophobicityRfMobility, HydrophobicityRoseAndOthers, HydrophobicityRoseman, HydrophobicityWellingAndOthers, HydrophobicityWolfendenAndOthers

Here is a complete list of available properties: ThreeLetterCode, OneLetterCode, AminoAcid, DNACodons, RNACodons, AcidicBasic, PolarNonpolar, Charged, Aromatic, HydrophobicHydophilic, IsoelectricPoint, pKCOOH, pKNH3+, ChemicalFormula, MolecularWeight, ExactMass, $Chemical Formula Minus H2O,\ Molecular Weight Minus H2O (18.01524),\ Exact Mass Minus H2O (18.01056),\ A substitution of the property of the$ vanderWaalsVolume, %AccessibleResidues, %BuriedResidues, AlphaHelixChouAndFasman, AlphaHelixDeleageAndRoux, AlphaHelixLevitt, AminoAcidsComposition, AminoAcidsCompositionInSwissProt, AntiparallelBetaStrand, AverageAreaBuried, AverageFlexibility, BetaSheetChouAndFasman, BetaSheetDeleageAndRoux, BetaSheetLevitt, BetaTurnChouAndFasman, BetaTurnDeleageAndRoux, BetaTurnLevitt, Bulkiness, CoilDeleageAndRoux, HPLCHFBARetention, HPLCRetentionAtpH2.1, HPLCRetentionAtpH7.4, HPLCTFARetention, HydrophobicityAbrahamAndLeo, HydrophobicityBlack, HydrophobicityBullAndBreese, HydrophobicityChothia, HydrophobicityEisenbergAndOthers, HydrophobicityFauchereAndOthers, HydrophobicityGuy, HydrophobicityHPLCAtpH3.4Cowan, HydrophobicityHPLCAtpH7.5Cowan, HydrophobicityHPLCParkerAndOthers, HydrophobicityHPLCWilsonAndOthers, HydrophobicityHoppAndWoods, HydrophobicityJanin, HydrophobicityKyteAndDoolittle, $Hydrophobicity Manavalan And Others,\ Hydrophobicity Miyazawa And Others,$ HydrophobicityOMHSweetAndOthers, HydrophobicityRaoAndArgos, HydrophobicityRfMobility, $Hydrophobicity Rose And Others,\ Hydrophobicity Roseman,\ Hydrophobicity Welling And Others,\ Hydrophobicity Rose And Others,\ Hyd$ HydrophobicityWolfendenAndOthers, ParallelBetaStrand, PolarityGrantham, PolarityZimmerman, RatioHeteroEndToSide, RecognitionFactors, Refractivity, RelativeMutability, TotalBetaStrand, LinearStructure, LinearStructureAtpH7.4

--propertieslisting ByGroup | Alphabetical

Specify how to list properties for amino 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: AminoAcidInfo<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 amino acid Ala, type:

% InfoAminoAcids.pl

To list all available properties information for amino acid Ala, type:

% InfoAminoAcids.pl --propertiesmode all

To list basic properties information for amino acids Ala, Arg, and Asp type:

```
% InfoAminoAcids.pl Ala Arg Asp
% InfoAminoAcids.pl A Arg "Aspartic acid"
```

To list all available properties information for amino acids Ala, Arg, and Asp type:

% InfoAminoAcids.pl --propertiesmode all Ala Arg Asp

To list basic and hydrophobicty properties information for amino acids Ala, Arg, and Asp type:

```
% InfoAminoAcids.pl --propertiesmode Categories
  --properties BasicAndHydrophobicity Ala Arg Asp
```

To list OneLetterCode, ThreeLetterCode, DNACodons, and MolecularWeight for amino acids Ala, Arg, and Asp type:

```
% InfoAminoAcids.pl --propertiesmode Names
   --properties OneLetterCode,ThreeLetterCode,DNACodons,MolecularWeight
Ala Arg Asp
```

To alphabetically list basic and hydrophobicty properties information for amino acids Ala, Arg, and Asp in rows insetad of amino acid blocks with quotes around the values, type:

```
% InfoAminoAcids.pl --propertiesmode Categories
   --properties BasicAndHydrophobicity --propertieslisting alphabetical
   --outdelim comma --outputstyle AminoAcidRows --quote yes Ala Arg Asp
```

To alphabetically list basic and hydrophobicty properties information for amino acids Ala, Arg, and Asp in rows insetad of amino acid blocks with quotes around the values and write them into a file AminoAcidProperties.csv, type:

```
% InfoAminoAcids.pl --propertiesmode Categories
   --properties BasicAndHydrophobicity --propertieslisting alphabetical
   --outdelim comma --outputstyle AminoAcidRows --quote yes
   --output File -r AminoAcidProperties -o Ala Arg Asp
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

 $InfoNucleicAcids.pl\ InfoPeriodicTableElements.pl$

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