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

AminoAcidIDs *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 *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, ChemicalFormulaMinusH2O, MolecularWeightMinusH2O(18.01524), ExactMassMinusH2O(18.01056), 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, HydrophobicityManavalanAndOthers, HydrophobicityMiyazawaAndOthers, HydrophobicityOMHSweetAndOthers, HydrophobicityRaoAndArgos, HydrophobicityRfMobility, HydrophobicityRoseAndOthers, HydrophobicityRoseman, HydrophobicityWellingAndOthers, 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
```

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SEE ALSO

InfoNucleicAcids.pl InfoPeriodicTableElements.pl

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