

## 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*, *HydrophobicHydrophilic*, *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*, *HydrophobicHydrophilic*, *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*, *HPLCHFARRetention*, *HPLCRetentionAtpH2.1*, *HPLCRetentionAtpH7.4*, *HPLCTFARRetention*, *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 hydrophobicity 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 hydrophobicity properties information for amino acids Ala, Arg, and Asp in rows instead 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 hydrophobicity properties information for amino acids Ala, Arg, and Asp in rows instead 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

## COPYRIGHT

Copyright (C) 2022 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.