Package: Interpol (via r-universe)

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Type Package

Title Interpolation of Amino Acid Sequences

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Description Numerical encoding as well as linear and non-linear interpolation of amino acid sequences. Compatibility updates by Renova.

License GPL (>= 2)

LazyLoad yes

Depends R (>= 2.10.0)

Repository https://renova-r.r-universe.dev

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AAdescriptor *AAdescriptor: Descriptor encoding of amino acids*

Description

Encodes amino acids into numerical values using descriptors.

Usage

```
AAdescriptor(data, descriptor = 151, normalize = 0)
```

Arguments

data	vector of protein sequences (as characters)
descriptor	descriptor to be used (range 1-532)
normalize	0: no normalization; 1:[-1,1]; 2:[0,1]

Value

returns the encoded (and normalized) amino acid sequences.

Author(s)

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References

Heider D., Hauke S., Pyka M., Kessler D. Advances and Applications in Bioinformatics and Chemistry 2010, 3:15-24

Kawashima, S.; Ogata, H.; Kanehisa, M. Nucleic Acids Res 1999, 27:368.

Examples

```
#### Amino acid sequence
a = c("MEGHIK", "MILIK")

#### encoding of sequence a with descriptor 151 and without normalization
b = AAdescriptor(a, 151, 0)
```

AAindex *AAindex database*

Description

The modified AAindex database with 533 descriptors for the twenty amino acids.

Usage

```
data(AAindex)
```

Details

1 alpha-CH_chemical_shifts_(Andersen_et_al.,_1992)

2 Hydrophobicity_index_(Argos_et_al.,_1982)

3 Signal_sequence_helical_potential_(Argos_et_al.,_1982)

4 Membrane-buried_preference_parameters_(Argos_et_al.,_1982)

5 Conformational_parameter_of_inner_helix_(Beghin-Dirkx,_1975)

6 Conformational_parameter_of_beta-structure_(Beghin-Dirkx,_1975)

7 Conformational_parameter_of_beta-turn_(Beghin-Dirkx,_1975)

8 Average_flexibility_indices_(Bhaskaran-Ponnuswamy,_1988)

9 Residue_volume_(Bigelow,_1967)

10 Information_value_for_accessibility;_average_fraction_35

11 Information_value_for_accessibility;_average_fraction_23

12 Retention_coefficient_in_TFA_(Browne_et_al.,_1982)

13 Retention_coefficient_in_HFBA_(Browne_et_al.,_1982)

14 Transfer_free_energy_to_surface_(Bull-Breese,_1974)

15 Apparent_partial_specific_volume_(Bull-Breese,_1974)

16 alpha-NH_chemical_shifts_(Bundi-Wuthrich,_1979)

17 alpha-CH_chemical_shifts_(Bundi-Wuthrich,_1979)

18 Spin-spin_coupling_constants_3JHalpha-NH_(Bundi-Wuthrich,_1979)

19 Normalized_frequency_of_alpha-helix_(Burgess_et_al.,_1974)

20 Normalized_frequency_of_extended_structure_(Burgess_et_al.,_1974)

21 Steric_parameter_(Charton,_1981)

22 Polarizability_parameter_(Charton-Charton,_1982)

23 Free_energy_of_solution_in_water,_kcal/mole_(Charton-Charton,_1982)

24 The_Chou-Fasman_parameter_of_the_coil_conformation_(Charton-Charton,_1983)

25 A_parameter_defined_from_the_residuals_obtained_from_the_best_correlation_of_the_Chou-Fasman_parameter_of_be
sheet_(Charton-Charton,_1983)

26 The_number_of_atoms_in_the_side_chain_labelled_1+1_(Charton-Charton,_1983)
27 The_number_of_atoms_in_the_side_chain_labelled_2+1_(Charton-Charton,_1983)
28 The_number_of_atoms_in_the_side_chain_labelled_3+1_(Charton-Charton,_1983)
29 The_number_of_bonds_in_the_longest_chain_(Charton-Charton,_1983)
30 A_parameter_of_charge_transfer_capability_(Charton-Charton,_1983)
31 A_parameter_of_charge_transfer_donor_capability_(Charton-Charton,_1983)
32 Average_volume_of_buried_residue_(Chothia,_1975)
33 Residue_accessible_surface_area_in_tripeptide_(Chothia,_1976)
34 Residue_accessible_surface_area_in_folded_protein_(Chothia,_1976)
35 Proportion_of_residues_95
36 Proportion_of_residues_100
37 Normalized_frequency_of_beta-turn_(Chou-Fasman,_1978a)
38 Normalized_frequency_of_alpha-helix_(Chou-Fasman,_1978b)
39 Normalized_frequency_of_beta-sheet_(Chou-Fasman,_1978b)
40 Normalized_frequency_of_beta-turn_(Chou-Fasman,_1978b)
41 Normalized_frequency_of_N-terminal_helix_(Chou-Fasman,_1978b)
42 Normalized_frequency_of_C-terminal_helix_(Chou-Fasman,_1978b)
43 Normalized_frequency_of_N-terminal_non_helical_region_(Chou-Fasman,_1978b)
44 Normalized_frequency_of_C-terminal_non_helical_region_(Chou-Fasman,_1978b)
45 Normalized_frequency_of_N-terminal_beta-sheet_(Chou-Fasman,_1978b)
46 Normalized_frequency_of_C-terminal_beta-sheet_(Chou-Fasman,_1978b)
47 Normalized_frequency_of_N-terminal_non_beta_region_(Chou-Fasman,_1978b)
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57 Normalized_hydrophobicity_scales_for_alpha/beta-proteins_(Cid_et_al.,_1992)
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72 Molecular_weight_(Fasman,_1976)
73 Melting_point_(Fasman,_1976)
74 Optical_rotation_(Fasman,_1976)
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76 pK-C_(Fasman,_1976)
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89 Negative_charge_(Fauchere_et_al.,_1988)
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91 Helix-coil_equilibrium_constant_(Finkelstein-Ptitsyn,_1977)
92 Helix_initiation_parameter_at_posision_i-1_(Finkelstein_et_al.,_1991)
93 Helix_initiation_parameter_at_posision_i,i+1,i+2_(Finkelstein_et_al.,_1991)
94 Helix_termination_parameter_at_posision_j-2,j-1,j_(Finkelstein_et_al.,_1991)
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111 Polarity_(Grantham,_1974)
112 Volume_(Grantham,_1974)
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114 Hydration_number_(Hopfinger,_1971),_Cited_by_Charton-Charton_(1982)
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123 Normalized_relative_frequency_of_bend_S_(Isogai_et_al.,_1980)
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130 Ratio_of_buried_and_accessible_molar_fractions_(Janin,_1979)
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155 Side_chain_angle_theta(AAR)_(Levitt,_1976)
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177 Refractivity_(McMeekin_et_al.,_1964),_Cited_by_Jones_(1975)
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179 Retention_coefficient_in_HPLC,_pH2.1_(Meek,_1980)
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181 Retention_coefficient_in_NaH2PO4_(Meek-Rossetti,_1981)
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183 Average_reduced_distance_for_side_chain_(Meirovitch_et_al.,_1980)
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211 14
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`Interpol` *Interpolation of encoded amino acid sequences*

Description

Interpolation of encoded protein sequences to a specific length. Interpol can be used to transform protein sequences to uniform length for subsequent classification.

Usage

```
Interpol(data, dims, method = "linear")
```

Arguments

`data`	list of encoded protein sequences (as numerical vectors)
`dims`	interpolation value (desired dimensionality)
`method`	"linear": linear interpolation "spline": cubic spline interpolation "natural": fulfills natural boundary conditions "periodic": fulfills periodic boundary conditions "fmm": interpolation of Forsythe "average": interval based averaging

Value

returns the interpolated encoded amino acid sequences with desired dimensionality.

Author(s)

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References

Heider D., Verheyen J., Hoffmann D.: Machine learning on normalized protein sequences, BMC Research Notes 2011, 4:94.

Examples

```
#### V3 data
data(V3)
sequence = V3[1]

#### encoding of sequence a with descriptor 151 and with normalization [0,1]
b = AAdescriptor(sequence, 151, 2)
b

#### interpolation to length 27 with linear interpolation
c = Interpol(b, 27, "linear")
c

#### plotting
plot(unlist(b), type="l", col="darkgreen", ylim=c(-3,3), ylab="descriptor value", xlab="sequence position", lwd=
lines(seq(1,length(unlist(b)),(length(unlist(b))/length(as.vector(c)))),as.vector(c), col="red", lwd=2)
axis(3, at=seq(1,35, 35/27), labels=1:27)
```

V3 *HIV-1 V3 loop dataset for tropism prediction*

Description

HIV-1 V3 loop dataset containing V3 sequences of 200 X4 and 1151 R5 viruses.

Usage

```
data(V3)
```

References

Dybowski J.N., Heider D., Hoffmann D. PLoS Computational Biology 2010, 6(4): e1000743.

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