Package 'Interpol'

February 19, 2015

Type Package

Title Interpolation of amino acid sequences

Version 1.3.1

Date 2011-07-08

Author Dominik Heider, PhD, University of Duisburg-Essen, Germany

Maintainer Dominik Heider <dominik.heider@uni-due.de>

Description A package for numerical encoding as well as for linear and non-linear interpolation of amino acid sequences.

License GPL (>= 2)

LazyLoad yes

Depends R (>= 2.10.0)

Repository CRAN

Date/Publication 2012-10-29 08:57:12

NeedsCompilation no

R topics documented:

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)

Dominik Heider, PhD, University of Duisburg-Essen, Germany

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)
48 Normalized_frequency_of_C-terminal_non_beta_region_(Chou-Fasman,_1978b)
49 Frequency_of_the_1st_residue_in_turn_(Chou-Fasman,_1978b)
50 Frequency_of_the_2nd_residue_in_turn_(Chou-Fasman,_1978b)
51 Frequency_of_the_3rd_residue_in_turn_(Chou-Fasman,_1978b)
52 Frequency_of_the_4th_residue_in_turn_(Chou-Fasman,_1978b)
53 Normalized_frequency_of_the_2nd_and_3rd_residues_in_turn_(Chou-Fasman,_1978b)
54 Normalized_hydrophobicity_scales_for_alpha-proteins_(Cid_et_al.,_1992)
55 Normalized_hydrophobicity_scales_for_beta-proteins_(Cid_et_al.,_1992)
56 Normalized_hydrophobicity_scales_for_alpha+beta-proteins_(Cid_et_al.,_1992)
57 Normalized_hydrophobicity_scales_for_alpha/beta-proteins_(Cid_et_al.,_1992)
58 Normalized_average_hydrophobicity_scales_(Cid_et_al.,_1992)
59 Partial_specific_volume_(Cohn-Edsall,_1943)
60 Normalized_frequency_of_middle_helix_(Crawford_et_al.,_1973)
61 Normalized_frequency_of_beta-sheet_(Crawford_et_al.,_1973)
62 Normalized_frequency_of_turn_(Crawford_et_al.,_1973)

63 Size_(Dawson,_1972)

64 Amino_acid_composition_(Dayhoff_et_al.,_1978a)

65 Relative_mutability_(Dayhoff_et_al.,_1978b)

66 Membrane_preference_for_cytochrome_b:_MPH89_(Degli_Esposti_et_al.,_1990)

67 Average_membrane_preference:_AMP07

68 Consensus_normalized_hydrophobicity_scale_(Eisenberg,_1984)

69 Solvation_free_energy_(Eisenberg-McLachlan,_1986)

70 Atom-based_hydrophobic_moment_(Eisenberg-McLachlan,_1986)

71 Direction_of_hydrophobic_moment_(Eisenberg-McLachlan,_1986)

72 Molecular_weight_(Fasman,_1976)

73 Melting_point_(Fasman,_1976)

74 Optical_rotation_(Fasman,_1976)

75 pK-N_(Fasman,_1976)

76 pK-C_(Fasman,_1976)

77 Hydrophobic_parameter_pi_(Fauchere-Pliska,_1983)

78 Graph_shape_index_(Fauchere_et_al.,_1988)

79 Smoothed_upsilon_steric_parameter_(Fauchere_et_al.,_1988)

80 Normalized_van_der_Waals_volume_(Fauchere_et_al.,_1988)

81 STERIMOL_length_of_the_side_chain_(Fauchere_et_al.,_1988)

82 STERIMOL_minimum_width_of_the_side_chain_(Fauchere_et_al.,_1988)

83 STERIMOL_maximum_width_of_the_side_chain_(Fauchere_et_al.,_1988)

84 N.m.r._chemical_shift_of_alpha-carbon_(Fauchere_et_al.,_1988)

85 Localized_electrical_effect_(Fauchere_et_al.,_1988)

86 Number_of_hydrogen_bond_donors_(Fauchere_et_al.,_1988)

87 Number_of_full_nonbonding_orbitals_(Fauchere_et_al.,_1988)

88 Positive_charge_(Fauchere_et_al.,_1988)

89 Negative_charge_(Fauchere_et_al.,_1988)

90 pK-a(RCOOH)_(Fauchere_et_al.,_1988)

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)

95 Helix_termination_parameter_at_posision_j+1_(Finkelstein_et_al.,_1991)

96 Partition_coefficient_(Garel_et_al.,_1973)

97 Alpha-helix_indices_(Geisow-Roberts,_1980)

98 Alpha-helix_indices_for_alpha-proteins_(Geisow-Roberts,_1980)

99 Alpha-helix_indices_for_beta-proteins_(Geisow-Roberts,_1980)

100 Alpha-helix_indices_for_alpha/beta-proteins_(Geisow-Roberts,_1980)
101 Beta-strand_indices_(Geisow-Roberts,_1980)
102 Beta-strand_indices_for_beta-proteins_(Geisow-Roberts,_1980)
103 Beta-strand_indices_for_alpha/beta-proteins_(Geisow-Roberts,_1980)
104 Aperiodic_indices_(Geisow-Roberts,_1980)
105 Aperiodic_indices_for_alpha-proteins_(Geisow-Roberts,_1980)
106 Aperiodic_indices_for_beta-proteins_(Geisow-Roberts,_1980)
107 Aperiodic_indices_for_alpha/beta-proteins_(Geisow-Roberts,_1980)
108 Hydrophobicity_factor_(Goldsack-Chalifoux,_1973)
109 Residue_volume_(Goldsack-Chalifoux,_1973)
110 Composition_(Grantham,_1974)
111 Polarity_(Grantham,_1974)
112 Volume_(Grantham,_1974)
113 Partition_energy_(Guy,_1985)
114 Hydration_number_(Hopfinger,_1971),_Cited_by_Charton-Charton_(1982)
115 Hydrophilicity_value_(Hopp-Woods,_1981)
116 Heat_capacity_(Hutchens,_1970)
117 Absolute_entropy_(Hutchens,_1970)
118 Entropy_of_formation_(Hutchens,_1970)
119 Normalized_relative_frequency_of_alpha-helix_(Isogai_et_al.,_1980)
120 Normalized_relative_frequency_of_extended_structure_(Isogai_et_al.,_1980)
121 Normalized_relative_frequency_of_bend_(Isogai_et_al.,_1980)
122 Normalized_relative_frequency_of_bend_R_(Isogai_et_al.,_1980)
123 Normalized_relative_frequency_of_bend_S_(Isogai_et_al.,_1980)
124 Normalized_relative_frequency_of_helix_end_(Isogai_et_al.,_1980)
125 Normalized_relative_frequency_of_double_bend_(Isogai_et_al.,_1980)
126 Normalized_relative_frequency_of_coil_(Isogai_et_al.,_1980)
127 Average_accessible_surface_area_(Janin_et_al.,_1978)
128 Percentage_of_buried_residues_(Janin_et_al.,_1978)
129 Percentage_of_exposed_residues_(Janin_et_al.,_1978)
130 Ratio_of_buried_and_accessible_molar_fractions_(Janin,_1979)
131 Transfer_free_energy_(Janin,_1979)
132 Hydrophobicity_(Jones,_1975)
133 pK_(-COOH)_(Jones,_1975)
134 Relative_frequency_of_occurrence_(Jones_et_al.,_1992)
135 Relative_mutability_(Jones_et_al.,_1992)
136 Amino_acid_distribution_(Jukes_et_al.,_1975)

137 Sequence_frequency_(Jungck,_1978)
138 Average_relative_probability_of_helix_(Kanehisa-Tsong,_1980)
139 Average_relative_probability_of_beta-sheet_(Kanehisa-Tsong,_1980)
140 Average_relative_probability_of_inner_helix_(Kanehisa-Tsong,_1980)
141 Average_relative_probability_of_inner_beta-sheet_(Kanehisa-Tsong,_1980)
142 Flexibility_parameter_for_no_rigid_neighbors_(Karplus-Schulz,_1985)
143 Flexibility_parameter_for_one_rigid_neighbor_(Karplus-Schulz,_1985)
144 Flexibility_parameter_for_two_rigid_neighbors_(Karplus-Schulz,_1985)
145 The_Kerr-constant_increments_(Khanarian-Moore,_1980)
146 Net_charge_(Klein_et_al.,_1984)
147 Side_chain_interaction_parameter_(Krigbaum-Rubin,_1971)
148 Side_chain_interaction_parameter_(Krigbaum-Komoriya,_1979)
149 Fraction_of_site_occupied_by_water_(Krigbaum-Komoriya,_1979)
150 Side_chain_volume_(Krigbaum-Komoriya,_1979)
151 Hydropathy_index_(Kyte-Doolittle,_1982)
152 Transfer_free_energy,_CHP/water_(Lawson_et_al.,_1984)
153 Hydrophobic_parameter_(Levitt,_1976)
154 Distance_between_C-alpha_and_centroid_of_side_chain_(Levitt,_1976)
155 Side_chain_angle_theta(AAR)_(Levitt,_1976)
156 Side_chain_torsion_angle_phi(AAAR)_(Levitt,_1976)
157 Radius_of_gyration_of_side_chain_(Levitt,_1976)
158 van_der_Waals_parameter_R0_(Levitt,_1976)
159 van_der_Waals_parameter_epsilon_(Levitt,_1976)
160 Normalized_frequency_of_alpha-helix,_with_weights_(Levitt,_1978)
161 Normalized_frequency_of_beta-sheet,_with_weights_(Levitt,_1978)
162 Normalized_frequency_of_reverse_turn,_with_weights_(Levitt,_1978)
163 Normalized_frequency_of_alpha-helix,_unweighted_(Levitt,_1978)
164 Normalized_frequency_of_beta-sheet,_unweighted_(Levitt,_1978)
165 Normalized_frequency_of_reverse_turn,_unweighted_(Levitt,_1978)
166 Frequency_of_occurrence_in_beta-bends_(Lewis_et_al.,_1971)
167 Conformational_preference_for_all_beta-strands_(Lifson-Sander,_1979)
168 Conformational_preference_for_parallel_beta-strands_(Lifson-Sander,_1979)
169 Conformational_preference_for_antiparallel_beta-strands_(Lifson-Sander,_1979)
170 Average_surrounding_hydrophobicity_(Manavalan-Ponnuswamy,_1978)
171 Normalized_frequency_of_alpha-helix_(Maxfield-Scheraga,_1976)
172 Normalized_frequency_of_extended_structure_(Maxfield-Scheraga,_1976)
173 Normalized_frequency_of_zeta_R_(Maxfield-Scheraga,_1976)

174 Normalized_frequency_of_left-handed_alpha-helix_(Maxfield-Scheraga,_1976)
175 Normalized_frequency_of_zeta_L_(Maxfield-Scheraga,_1976)
176 Normalized_frequency_of_alpha_region_(Maxfield-Scheraga,_1976)
177 Refractivity_(McMeekin_et_al.,_1964),_Cited_by_Jones_(1975)
178 Retention_coefficient_in_HPLC,_pH7.4_(Meek,_1980)
179 Retention_coefficient_in_HPLC,_pH2.1_(Meek,_1980)
180 Retention_coefficient_in_NaClO4_(Meek-Rossetti,_1981)
181 Retention_coefficient_in_NaH2PO4_(Meek-Rossetti,_1981)
182 Average_reduced_distance_for_C-alpha_(Meirovitch_et_al.,_1980)
183 Average_reduced_distance_for_side_chain_(Meirovitch_et_al.,_1980)
184 Average_side_chain_orientation_angle_(Meirovitch_et_al.,_1980)
185 Effective_partition_energy_(Miyazawa-Jernigan,_1985)
186 Normalized_frequency_of_alpha-helix_(Nagano,_1973)
187 Normalized_frequency_of_bata-structure_(Nagano,_1973)
188 Normalized_frequency_of_coil_(Nagano,_1973)
189 AA_composition_of_total_proteins_(Nakashima_et_al.,_1990)
190 SD_of_AA_composition_of_total_proteins_(Nakashima_et_al.,_1990)
191 AA_composition_of_mt-proteins_(Nakashima_et_al.,_1990)
192 Normalized_composition_of_mt-proteins_(Nakashima_et_al.,_1990)
193 AA_composition_of_mt-proteins_from_animal_(Nakashima_et_al.,_1990)
194 Normalized_composition_from_animal_(Nakashima_et_al.,_1990)
195 AA_composition_of_mt-proteins_from_fungi_and_plant_(Nakashima_et_al.,_1990)
196 Normalized_composition_from_fungi_and_plant_(Nakashima_et_al.,_1990)
197 AA_composition_of_membrane_proteins_(Nakashima_et_al.,_1990)
198 Normalized_composition_of_membrane_proteins_(Nakashima_et_al.,_1990)
199 Transmembrane_regions_of_non-mt-proteins_(Nakashima_et_al.,_1990)
200 Transmembrane_regions_of_mt-proteins_(Nakashima_et_al.,_1990)
201 Ratio_of_average_and_computed_composition_(Nakashima_et_al.,_1990)
202 AA_composition_of_CYT_of_single-spanning_proteins_(Nakashima-Nishikawa,_1992)
203 AA_composition_of_CYT2_of_single-spanning_proteins_(Nakashima-Nishikawa,_1992)
204 AA_composition_of_EXT_of_single-spanning_proteins_(Nakashima-Nishikawa,_1992)
205 AA_composition_of_EXT2_of_single-spanning_proteins_(Nakashima-Nishikawa,_1992)
206 AA_composition_of_MEM_of_single-spanning_proteins_(Nakashima-Nishikawa,_1992)
207 AA_composition_of_CYT_of_multi-spanning_proteins_(Nakashima-Nishikawa,_1992)
208 AA_composition_of_EXT_of_multi-spanning_proteins_(Nakashima-Nishikawa,_1992)
209 AA_composition_of_MEM_of_multi-spanning_proteins_(Nakashima-Nishikawa,_1992)
210 8_A_contact_number_(Nishikawa-Ooi,_1980)

211 14
212 Transfer_energy,_organic_solvent/water_(Nozaki-Tanford,_1971)
213 Average_non-bonded_energy_per_atom_(Oobatake-Ooi,_1977)
214 Short_and_medium_range_non-bonded_energy_per_atom_(Oobatake-Ooi,_1977)
215 Long_range_non-bonded_energy_per_atom_(Oobatake-Ooi,_1977)
216 Average_non-bonded_energy_per_residue_(Oobatake-Ooi,_1977)
217 Short_and_medium_range_non-bonded_energy_per_residue_(Oobatake-Ooi,_1977)
218 Optimized_beta-structure-coil_equilibrium_constant_(Oobatake_et_al.,_1985)
219 Optimized_propensity_to_form_reverse_turn_(Oobatake_et_al.,_1985)
220 Optimized_transfer_energy_parameter_(Oobatake_et_al.,_1985)
221 Optimized_average_non-bonded_energy_per_atom_(Oobatake_et_al.,_1985)
222 Optimized_side_chain_interaction_parameter_(Oobatake_et_al.,_1985)
223 Normalized_frequency_of_alpha-helix_from_LG_(Palau_et_al.,_1981)
224 Normalized_frequency_of_alpha-helix_from_CF_(Palau_et_al.,_1981)
225 Normalized_frequency_of_beta-sheet_from_LG_(Palau_et_al.,_1981)
226 Normalized_frequency_of_beta-sheet_from_CF_(Palau_et_al.,_1981)
227 Normalized_frequency_of_turn_from_LG_(Palau_et_al.,_1981)
228 Normalized_frequency_of_turn_from_CF_(Palau_et_al.,_1981)
229 Normalized_frequency_of_alpha-helix_in_all-alpha_class_(Palau_et_al.,_1981)
230 Normalized_frequency_of_alpha-helix_in_alpha+beta_class_(Palau_et_al.,_1981)
231 Normalized_frequency_of_alpha-helix_in_alpha/beta_class_(Palau_et_al.,_1981)
232 Normalized_frequency_of_beta-sheet_in_all-beta_class_(Palau_et_al.,_1981)
233 Normalized_frequency_of_beta-sheet_in_alpha+beta_class_(Palau_et_al.,_1981)
234 Normalized_frequency_of_beta-sheet_in_alpha/beta_class_(Palau_et_al.,_1981)
235 Normalized_frequency_of_turn_in_all-alpha_class_(Palau_et_al.,_1981)
236 Normalized_frequency_of_turn_in_all-beta_class_(Palau_et_al.,_1981)
237 Normalized_frequency_of_turn_in_alpha+beta_class_(Palau_et_al.,_1981)
238 Normalized_frequency_of_turn_in_alpha/beta_class_(Palau_et_al.,_1981)
239 HPLC_parameter_(Parker_et_al.,_1986)
240 Partition_coefficient_(Pliska_et_al.,_1981)
241 Surrounding_hydrophobicity_in_folded_form_(Ponnuswamy_et_al.,_1980)
242 Average_gain_in_surrounding_hydrophobicity_(Ponnuswamy_et_al.,_1980)
243 Average_gain_ratio_in_surrounding_hydrophobicity_(Ponnuswamy_et_al.,_1980)
244 Surrounding_hydrophobicity_in_alpha-helix_(Ponnuswamy_et_al.,_1980)
245 Surrounding_hydrophobicity_in_beta-sheet_(Ponnuswamy_et_al.,_1980)
246 Surrounding_hydrophobicity_in_turn_(Ponnuswamy_et_al.,_1980)
247 Accessibility_reduction_ratio_(Ponnuswamy_et_al.,_1980)

248 Average_number_of_surrounding_residues_(Ponnuswamy_et_al.,_1980)
249 Intercept_in_regression_analysis_(Prabhakaran-Ponnuswamy,_1982)
250 Slope_in_regression_analysis_x_1.0E1_(Prabhakaran-Ponnuswamy,_1982)
251 Correlation_coefficient_in_regression_analysis_(Prabhakaran-Ponnuswamy,_1982)
252 Hydrophobicity_(Prabhakaran,_1990)
253 Relative_frequency_in_alpha-helix_(Prabhakaran,_1990)
254 Relative_frequency_in_beta-sheet_(Prabhakaran,_1990)
255 Relative_frequency_in_reverse-turn_(Prabhakaran,_1990)
256 Helix-coil_equilibrium_constant_(Ptitsyn-Finkelstein,_1983)
257 Beta-coil_equilibrium_constant_(Ptitsyn-Finkelstein,_1983)
258 Weights_for_alpha-helix_at_the_window_position_of_-6_(Qian-Sejnowski,_1988)
259 Weights_for_alpha-helix_at_the_window_position_of_-5_(Qian-Sejnowski,_1988)
260 Weights_for_alpha-helix_at_the_window_position_of_-4_(Qian-Sejnowski,_1988)
261 Weights_for_alpha-helix_at_the_window_position_of_-3_(Qian-Sejnowski,_1988)
262 Weights_for_alpha-helix_at_the_window_position_of_-2_(Qian-Sejnowski,_1988)
263 Weights_for_alpha-helix_at_the_window_position_of_-1_(Qian-Sejnowski,_1988)
264 Weights_for_alpha-helix_at_the_window_position_of_0_(Qian-Sejnowski,_1988)
265 Weights_for_alpha-helix_at_the_window_position_of_1_(Qian-Sejnowski,_1988)
266 Weights_for_alpha-helix_at_the_window_position_of_2_(Qian-Sejnowski,_1988)
267 Weights_for_alpha-helix_at_the_window_position_of_3_(Qian-Sejnowski,_1988)
268 Weights_for_alpha-helix_at_the_window_position_of_4_(Qian-Sejnowski,_1988)
269 Weights_for_alpha-helix_at_the_window_position_of_5_(Qian-Sejnowski,_1988)
270 Weights_for_alpha-helix_at_the_window_position_of_6_(Qian-Sejnowski,_1988)
271 Weights_for_beta-sheet_at_the_window_position_of_-6_(Qian-Sejnowski,_1988)
272 Weights_for_beta-sheet_at_the_window_position_of_-5_(Qian-Sejnowski,_1988)
273 Weights_for_beta-sheet_at_the_window_position_of_-4_(Qian-Sejnowski,_1988)
274 Weights_for_beta-sheet_at_the_window_position_of_-3_(Qian-Sejnowski,_1988)
275 Weights_for_beta-sheet_at_the_window_position_of_-2_(Qian-Sejnowski,_1988)
276 Weights_for_beta-sheet_at_the_window_position_of_-1_(Qian-Sejnowski,_1988)
277 Weights_for_beta-sheet_at_the_window_position_of_0_(Qian-Sejnowski,_1988)
278 Weights_for_beta-sheet_at_the_window_position_of_1_(Qian-Sejnowski,_1988)
279 Weights_for_beta-sheet_at_the_window_position_of_2_(Qian-Sejnowski,_1988)
280 Weights_for_beta-sheet_at_the_window_position_of_3_(Qian-Sejnowski,_1988)
281 Weights_for_beta-sheet_at_the_window_position_of_4_(Qian-Sejnowski,_1988)
282 Weights_for_beta-sheet_at_the_window_position_of_5_(Qian-Sejnowski,_1988)
283 Weights_for_beta-sheet_at_the_window_position_of_6_(Qian-Sejnowski,_1988)
284 Weights_for_coil_at_the_window_position_of_-6_(Qian-Sejnowski,_1988)

285 Weights_for_coil_at_the_window_position_of_-5_(Qian-Sejnowski,_1988)
286 Weights_for_coil_at_the_window_position_of_-4_(Qian-Sejnowski,_1988)
287 Weights_for_coil_at_the_window_position_of_-3_(Qian-Sejnowski,_1988)
288 Weights_for_coil_at_the_window_position_of_-2_(Qian-Sejnowski,_1988)
289 Weights_for_coil_at_the_window_position_of_-1_(Qian-Sejnowski,_1988)
290 Weights_for_coil_at_the_window_position_of_0_(Qian-Sejnowski,_1988)
291 Weights_for_coil_at_the_window_position_of_1_(Qian-Sejnowski,_1988)
292 Weights_for_coil_at_the_window_position_of_2_(Qian-Sejnowski,_1988)
293 Weights_for_coil_at_the_window_position_of_3_(Qian-Sejnowski,_1988)
294 Weights_for_coil_at_the_window_position_of_4_(Qian-Sejnowski,_1988)
295 Weights_for_coil_at_the_window_position_of_5_(Qian-Sejnowski,_1988)
296 Weights_for_coil_at_the_window_position_of_6_(Qian-Sejnowski,_1988)
297 Average_reduced_distance_for_C-alpha_(Rackovsky-Scheraga,_1977)
298 Average_reduced_distance_for_side_chain_(Rackovsky-Scheraga,_1977)
299 Side_chain_orientational_preference_(Rackovsky-Scheraga,_1977)
300 Average_relative_fractional_occurrence_in_A0(i)_(Rackovsky-Scheraga,_1982)
301 Average_relative_fractional_occurrence_in_AR(i)_(Rackovsky-Scheraga,_1982)
302 Average_relative_fractional_occurrence_in_AL(i)_(Rackovsky-Scheraga,_1982)
303 Average_relative_fractional_occurrence_in_EL(i)_(Rackovsky-Scheraga,_1982)
304 Average_relative_fractional_occurrence_in_E0(i)_(Rackovsky-Scheraga,_1982)
305 Average_relative_fractional_occurrence_in_ER(i)_(Rackovsky-Scheraga,_1982)
306 Average_relative_fractional_occurrence_in_A0(i-1)_(Rackovsky-Scheraga,_1982)
307 Average_relative_fractional_occurrence_in_AR(i-1)_(Rackovsky-Scheraga,_1982)
308 Average_relative_fractional_occurrence_in_AL(i-1)_(Rackovsky-Scheraga,_1982)
309 Average_relative_fractional_occurrence_in_EL(i-1)_(Rackovsky-Scheraga,_1982)
310 Average_relative_fractional_occurrence_in_E0(i-1)_(Rackovsky-Scheraga,_1982)
311 Average_relative_fractional_occurrence_in_ER(i-1)_(Rackovsky-Scheraga,_1982)
312 Value_of_theta(i)_(Rackovsky-Scheraga,_1982)
313 Value_of_theta(i-1)_(Rackovsky-Scheraga,_1982)
314 Transfer_free_energy_from_chx_to_wat_(Radzicka-Wolfenden,_1988)
315 Transfer_free_energy_from_oct_to_wat_(Radzicka-Wolfenden,_1988)
316 Transfer_free_energy_from_vap_to_chx_(Radzicka-Wolfenden,_1988)
317 Transfer_free_energy_from_chx_to_oct_(Radzicka-Wolfenden,_1988)
318 Transfer_free_energy_from_vap_to_oct_(Radzicka-Wolfenden,_1988)
319 Accessible_surface_area_(Radzicka-Wolfenden,_1988)
320 Energy_transfer_from_out_to_in(95
321 Mean_polarity_(Radzicka-Wolfenden,_1988)

322 Relative_preference_value_at_N"_(Richardson-Richardson,_1988)
323 Relative_preference_value_at_N'_(Richardson-Richardson,_1988)
324 Relative_preference_value_at_N-cap_(Richardson-Richardson,_1988)
325 Relative_preference_value_at_N1_(Richardson-Richardson,_1988)
326 Relative_preference_value_at_N2_(Richardson-Richardson,_1988)
327 Relative_preference_value_at_N3_(Richardson-Richardson,_1988)
328 Relative_preference_value_at_N4_(Richardson-Richardson,_1988)
329 Relative_preference_value_at_N5_(Richardson-Richardson,_1988)
330 Relative_preference_value_at_Mid_(Richardson-Richardson,_1988)
331 Relative_preference_value_at_C5_(Richardson-Richardson,_1988)
332 Relative_preference_value_at_C4_(Richardson-Richardson,_1988)
333 Relative_preference_value_at_C3_(Richardson-Richardson,_1988)
334 Relative_preference_value_at_C2_(Richardson-Richardson,_1988)
335 Relative_preference_value_at_C1_(Richardson-Richardson,_1988)
336 Relative_preference_value_at_C-cap_(Richardson-Richardson,_1988)
337 Relative_preference_value_at_C'_(Richardson-Richardson,_1988)
338 Relative_preference_value_at_C"_(Richardson-Richardson,_1988)
339 Information_measure_for_alpha-helix_(Robson-Suzuki,_1976)
340 Information_measure_for_N-terminal_helix_(Robson-Suzuki,_1976)
341 Information_measure_for_middle_helix_(Robson-Suzuki,_1976)
342 Information_measure_for_C-terminal_helix_(Robson-Suzuki,_1976)
343 Information_measure_for_extended_(Robson-Suzuki,_1976)
344 Information_measure_for_pleated-sheet_(Robson-Suzuki,_1976)
345 Information_measure_for_extended_without_H-bond_(Robson-Suzuki,_1976)
346 Information_measure_for_turn_(Robson-Suzuki,_1976)
347 Information_measure_for_N-terminal_turn_(Robson-Suzuki,_1976)
348 Information_measure_for_middle_turn_(Robson-Suzuki,_1976)
349 Information_measure_for_C-terminal_turn_(Robson-Suzuki,_1976)
350 Information_measure_for_coil_(Robson-Suzuki,_1976)
351 Information_measure_for_loop_(Robson-Suzuki,_1976)
352 Hydration_free_energy_(Robson-Osguthorpe,_1979)
353 Mean_area_buried_on_transfer_(Rose_et_al.,_1985)
354 Mean_fractional_area_loss_(Rose_et_al.,_1985)
355 Side_chain_hydropathy,_uncorrected_for_solvation_(Roseman,_1988)
356 Side_chain_hydropathy,_corrected_for_solvation_(Roseman,_1988)
357 Loss_of_Side_chain_hydropathy_by_helix_formation_(Roseman,_1988)
358 Transfer_free_energy_(Simon,_1976),_Cited_by_Charton-Charton_(1982)

359 Principal_component_I_(Sneath,_1966)
360 Principal_component_II_(Sneath,_1966)
361 Principal_component_III_(Sneath,_1966)
362 Principal_component_IV_(Sneath,_1966)
363 Zimm-Bragg_parameter_s_at_20_C_(Sueki_et_al.,_1984)
364 Zimm-Bragg_parameter_sigma_x_1.0E4_(Sueki_et_al.,_1984)
365 Optimal_matching_hydrophobicity_(Sweet-Eisenberg,_1983)
366 Normalized_frequency_of_alpha-helix_(Tanaka-Scheraga,_1977)
367 Normalized_frequency_of_isolated_helix_(Tanaka-Scheraga,_1977)
368 Normalized_frequency_of_extended_structure_(Tanaka-Scheraga,_1977)
369 Normalized_frequency_of_chain_reversal_R_(Tanaka-Scheraga,_1977)
370 Normalized_frequency_of_chain_reversal_S_(Tanaka-Scheraga,_1977)
371 Normalized_frequency_of_chain_reversal_D_(Tanaka-Scheraga,_1977)
372 Normalized_frequency_of_left-handed_helix_(Tanaka-Scheraga,_1977)
373 Normalized_frequency_of_zeta_R_(Tanaka-Scheraga,_1977)
374 Normalized_frequency_of_coil_(Tanaka-Scheraga,_1977)
375 Normalized_frequency_of_chain_reversal_(Tanaka-Scheraga,_1977)
376 Relative_population_of_conformational_state_A_(Vasquez_et_al.,_1983)
377 Relative_population_of_conformational_state_C_(Vasquez_et_al.,_1983)
378 Relative_population_of_conformational_state_E_(Vasquez_et_al.,_1983)
379 Electron-ion_interaction_potential_(Veljkovic_et_al.,_1985)
380 Bitterness_(Venanzi,_1984)
381 Transfer_free_energy_to_lipophilic_phase_(von_Heijne-Blomberg,_1979)
382 Average_interactions_per_side_chain_atom_(Warme-Morgan,_1978)
383 RF_value_in_high_salt_chromatography_(Weber-Lacey,_1978)
384 Propensity_to_be_buried_inside_(Wertz-Scheraga,_1978)
385 Free_energy_change_of_epsilon(i)_to_epsilon(ex)_(Wertz-Scheraga,_1978)
386 Free_energy_change_of_alpha(Ri)_to_alpha(Rh)_(Wertz-Scheraga,_1978)
387 Free_energy_change_of_epsilon(i)_to_alpha(Rh)_(Wertz-Scheraga,_1978)
388 Polar_requirement_(Woese,_1973)
389 Hydration_potential_(Wolfenden_et_al.,_1981)
390 Principal_property_value_z1_(Wold_et_al.,_1987)
391 Principal_property_value_z2_(Wold_et_al.,_1987)
392 Principal_property_value_z3_(Wold_et_al.,_1987)
393 Unfolding_Gibbs_energy_in_water,_pH7.0_(Yutani_et_al.,_1987)
394 Unfolding_Gibbs_energy_in_water,_pH9.0_(Yutani_et_al.,_1987)
395 Activation_Gibbs_energy_of_unfolding,_pH7.0_(Yutani_et_al.,_1987)

396 Activation_Gibbs_energy_of_unfolding,_pH9.0_(Yutani_et_al.,_1987)
397 Dependence_of_partition_coefficient_on_ionic_strength_(Zaslavsky_et_al.,_1982)
398 Hydrophobicity_(Zimmerman_et_al.,_1968)
399 Bulkiness_(Zimmerman_et_al.,_1968)
400 Polarity_(Zimmerman_et_al.,_1968)
401 Isoelectric_point_(Zimmerman_et_al.,_1968)
402 RF_rank_(Zimmerman_et_al.,_1968)
403 Normalized_positional_residue_frequency_at_helix_termini_N4’(Aurora-Rose,_1998)
404 Normalized_positional_residue_frequency_at_helix_termini_N"’_(Aurora-Rose,_1998)
405 Normalized_positional_residue_frequency_at_helix_termini_N"_(Aurora-Rose,_1998)
406 Normalized_positional_residue_frequency_at_helix_termini_N’(Aurora-Rose,_1998)
407 Normalized_positional_residue_frequency_at_helix_termini_Nc_(Aurora-Rose,_1998)
408 Normalized_positional_residue_frequency_at_helix_termini_N1_(Aurora-Rose,_1998)
409 Normalized_positional_residue_frequency_at_helix_termini_N2_(Aurora-Rose,_1998)
410 Normalized_positional_residue_frequency_at_helix_termini_N3_(Aurora-Rose,_1998)
411 Normalized_positional_residue_frequency_at_helix_termini_N4_(Aurora-Rose,_1998)
412 Normalized_positional_residue_frequency_at_helix_termini_N5_(Aurora-Rose,_1998)
413 Normalized_positional_residue_frequency_at_helix_termini_C5_(Aurora-Rose,_1998)
414 Normalized_positional_residue_frequency_at_helix_termini_C4_(Aurora-Rose,_1998)
415 Normalized_positional_residue_frequency_at_helix_termini_C3_(Aurora-Rose,_1998)
416 Normalized_positional_residue_frequency_at_helix_termini_C2_(Aurora-Rose,_1998)
417 Normalized_positional_residue_frequency_at_helix_termini_C1_(Aurora-Rose,_1998)
418 Normalized_positional_residue_frequency_at_helix_termini_Cc_(Aurora-Rose,_1998)
419 Normalized_positional_residue_frequency_at_helix_termini_C’_(Aurora-Rose,_1998)
420 Normalized_positional_residue_frequency_at_helix_termini_C"_(Aurora-Rose,_1998)
421 Normalized_positional_residue_frequency_at_helix_termini_C"’_(Aurora-Rose,_1998)
422 Normalized_positional_residue_frequency_at_helix_termini_C4’_(Aurora-Rose,_1998)
423 Delta_G_values_for_the_peptides_extrapolated_to_0_M_urea_(O’Neil-DeGrado,_1990)
424 Helix_formation_parameters_(delta_delta_G)_(O’Neil-DeGrado,_1990)
425 Normalized_flexibility_parameters_(B-values),_average_(Vihinen_et_al.,_1994)
426 Normalized_flexibility_parameters_(B-values)_for_each_residue_surrounded_by_none_rigid_neighbours_(Vihinen_et_
427 Normalized_flexibility_parameters_(B-values)_for_each_residue_surrounded_by_one_rigid_neighbours_(Vihinen_et_a
428 Normalized_flexibility_parameters_(B-values)_for_each_residue_surrounded_by_two_rigid_neighbours_(Vihinen_et_a
429 Free_energy_in_alpha-helical_conformation_(Munoz-Serrano,_1994)
430 Free_energy_in_alpha-helical_region_(Munoz-Serrano,_1994)
431 Free_energy_in_beta-strand_conformation_(Munoz-Serrano,_1994)
432 Free_energy_in_beta-strand_region_(Munoz-Serrano,_1994)

433 Free_energy_in_beta-strand_region_(Munoz-Serrano,_1994)

434 Free_energies_of_transfer_of_AcWl-X-LL_peptides_from_bilayer_interface_to_water_(Wimley-White,_1996)

435 Thermodynamic_beta_sheet_propensity_(Kim-Berg,_1993)

436 Turn_propensity_scale_for_transmembrane_helices_(Monne_et_al.,_1999)

437 Alpha_helix_propensity_of_position_44_in_T4_lysozyme_(Blaber_et_al.,_1993)

438 p-Values_of_mesophilic_proteins_based_on_the_distributions_of_B_values_(Parthasarathy-Murthy,_2000)

439 p-Values_of_thermophilic_proteins_based_on_the_distributions_of_B_values_(Parthasarathy-Murthy,_2000)

440 Distribution_of_amino_acid_residues_in_the_18_non-redundant_families_of_thermophilic_proteins_(Kumar_et_al.,_2

441 Distribution_of_amino_acid_residues_in_the_18_non-redundant_families_of_mesophilic_proteins_(Kumar_et_al.,_20

442 Distribution_of_amino_acid_residues_in_the_alpha-helices_in_thermophilic_proteins_(Kumar_et_al.,_2000)

443 Distribution_of_amino_acid_residues_in_the_alpha-helices_in_mesophilic_proteins_(Kumar_et_al.,_2000)

444 Side-chain_contribution_to_protein_stability_(kJ/mol)_(Takano-Yutani,_2001)

445 Propensity_of_amino_acids_within_pi-helices_(Fodje-Al-Karadaghi,_2002)

446 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(5

447 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(9

448 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(16

449 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(20

450 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(25

451 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(36

452 Hydropathy_scale_based_on_self-information_values_in_the_two-state_model_(50

453 Averaged_turn_propensities_in_a_transmembrane_helix_(Monne_et_al.,_1999)

454 Alpha-helix_propensity_derived_from_designed_sequences_(Koehl-Levitt,_1999)

455 Beta-sheet_propensity_derived_from_designed_sequences_(Koehl-Levitt,_1999)

456 Composition_of_amino_acids_in_extracellular_proteins_(percent)_(Cedano_et_al.,_1997)

457 Composition_of_amino_acids_in_anchored_proteins_(percent)_(Cedano_et_al.,_1997)

458 Composition_of_amino_acids_in_membrane_proteins_(percent)_(Cedano_et_al.,_1997)

459 Composition_of_amino_acids_in_intracellular_proteins_(percent)_(Cedano_et_al.,_1997)

460 Composition_of_amino_acids_in_nuclear_proteins_(percent)_(Cedano_et_al.,_1997)

461 Surface_composition_of_amino_acids_in_intracellular_proteins_of_thermophiles_(percent)_(Fukuchi-Nishikawa,_2001)

462 Surface_composition_of_amino_acids_in_intracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

463 Surface_composition_of_amino_acids_in_extracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

464 Surface_composition_of_amino_acids_in_nuclear_proteins_(percent)_(Fukuchi-Nishikawa,_2001)

465 Interior_composition_of_amino_acids_in_intracellular_proteins_of_thermophiles_(percent)_(Fukuchi-Nishikawa,_2001)

466 Interior_composition_of_amino_acids_in_intracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

467 Interior_composition_of_amino_acids_in_extracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

468 Interior_composition_of_amino_acids_in_nuclear_proteins_(percent)_(Fukuchi-Nishikawa,_2001)

469 Entire_chain_composition_of_amino_acids_in_intracellular_proteins_of_thermophiles_(percent)_(Fukuchi-Nishikawa,_2001)

470 Entire_chain_composition_of_amino_acids_in_intracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

471 Entire_chain_composition_of_amino_acids_in_extracellular_proteins_of_mesophiles_(percent)_(Fukuchi-Nishikawa,_2001)

472 Entire_chain_compositino_of_amino_acids_in_nuclear_proteins_(percent)_(Fukuchi-Nishikawa,_2001)

473 Amphiphilicity_index_(Mitaku_et_al.,_2002)

474 Volumes_including_the_crystallographic_waters_using_the_ProtOr_(Tsai_et_al.,_1999)

475 Volumes_not_including_the_crystallographic_waters_using_the_ProtOr_(Tsai_et_al.,_1999)

476 Electron-ion_interaction_potential_values_(Cosic,_1994)

477 Hydrophobicity_scales_(Ponnuswamy,_1993)

478 Hydrophobicity_coefficient_in_RP-HPLC,_C18_with_0.1

479 Hydrophobicity_coefficient_in_RP-HPLC,_C8_with_0.1

480 Hydrophobicity_coefficient_in_RP-HPLC,_C4_with_0.1

481 Hydrophobicity_coefficient_in_RP-HPLC,_C18_with_0.1

482 Hydrophilicity_scale_(Kuhn_et_al.,_1995)

483 Retention_coefficient_at_pH_2_(Guo_et_al.,_1986)

484 Modified_Kyte-Doolittle_hydrophobicity_scale_(Juretic_et_al.,_1998)

485 Interactivity_scale_obtained_from_the_contact_matrix_(Bastolla_et_al.,_2005)

486 Interactivity_scale_obtained_by_maximizing_the_mean_of_correlation_coefficient_over_single-domain_globular_proteins_(Bastolla_et_al.,_2005)

487 Interactivity_scale_obtained_by_maximizing_the_mean_of_correlation_coefficient_over_pairs_of_sequences_sharing_

488 Linker_propensity_index_(Suyama-Ohara,_2003)

489 Knowledge-based_membrane-propensity_scale_from_1D_Helix_in_MPtopo_databases_(Punta-Maritan,_2003)

490 Knowledge-based_membrane-propensity_scale_from_3D_Helix_in_MPtopo_databases_(Punta-Maritan,_2003)

491 Linker_propensity_from_all_dataset_(George-Heringa,_2003)

492 Linker_propensity_from_1-linker_dataset_(George-Heringa,_2003)

493 Linker_propensity_from_2-linker_dataset_(George-Heringa,_2003)

494 Linker_propensity_from_3-linker_dataset_(George-Heringa,_2003)

495 Linker_propensity_from_small_dataset_(linker_length_is_less_than_six_residues)_(George-Heringa,_2003)
496 Linker_propensity_from_medium_dataset_(linker_length_is_between_six_and_14
497 Linker_propensity_from_long_dataset_(linker_length_is_greater_than_14
498 Linker_propensity_from_helical_(annotated_by_DSSP)_dataset_(George-Heringa,_2003)
499 Linker_propensity_from_non-helical_(annotated_by_DSSP)_dataset_(George-Heringa,_2003)
500 The_stability_scale_from_the_knowledge-based_atom-atom_potential_(Zhou-Zhou,_2004)
501 The_relative_stability_scale_extracted_from_mutation_experiments_(Zhou-Zhou,_2004)
502 Buriability_(Zhou-Zhou,_2004)
503 Linker_index_(Bae_et_al.,_2005)
504 Mean_volumes_of_residues_buried_in_protein_interiors_(Harpaz_et_al.,_1994)
505 Average_volumes_of_residues_(Pontius_et_al.,_1996)
506 Hydrostatic_pressure_asymmetry_index,_PAI_(Di_Giulio,_2005)
507 Hydrophobicity_index_(Wolfenden_et_al.,_1979)
508 Average_internal_preferences_(Olsen,_1980)
509 Hydrophobicity-related_index_(Kidera_et_al.,_1985)
510 Apparent_partition_energies_calculated_from_Wertz-Scheraga_index_(Guy,_1985)
511 Apparent_partition_energies_calculated_from_Janin_index_(Guy,_1985)
512 Apparent_partition_energies_calculated_from_Chothia_index_(Guy,_1985)
513 Weights_from_the_IFH_scale_(Jacobs-White,_1989)
514 Hydrophobicity_index,_3.0_pH_(Cowan-Whittaker,_1990)
515 Scaled_side_chain_hydrophobicity_values_(Black-Mould,_1991)
516 Hydrophobicity_scale_from_native_protein_structures_(Casari-Sippl,_1992)
517 NNEIG_index_(Cornette_et_al.,_1987)
518 SWEIG_index_(Cornette_et_al.,_1987)
519 PRIFT_index_(Cornette_et_al.,_1987)
520 PRILS_index_(Cornette_et_al.,_1987)
521 ALTFT_index_(Cornette_et_al.,_1987)
522 ALTLS_index_(Cornette_et_al.,_1987)
523 TOTFT_index_(Cornette_et_al.,_1987)
524 TOTLS_index_(Cornette_et_al.,_1987)
525 Relative_partition_energies_derived_by_the_Bethe_approximation_(Miyazawa-Jernigan,_1999)
526 Optimized_relative_partition_energies_-_method_A_(Miyazawa-Jernigan,_1999)
527 Optimized_relative_partition_energies_-_method_B_(Miyazawa-Jernigan,_1999)
528 Optimized_relative_partition_energies_-_method_C_(Miyazawa-Jernigan,_1999)
529 Optimized_relative_partition_energies_-_method_D_(Miyazawa-Jernigan,_1999)
530 Hydrophobicity_index_(Engelman_et_al.,_1986)
531 Hydrophobicity_index_(Fasman,_1989)
532 GA_APV_OUT_(Heider,_Nov_2010)
533 GAD_(Heider_et_al.,_2011)

References

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

`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)

Dominik Heider, PhD, University of Duisburg-Essen, Germany

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.

Index