

# Indices—Features That Represents Clusters

- 1 — Normalized frequency of chain reversal R (Tanaka-Scheraga, 1977)
- 2 — Linker propensity from non-helical (annotated by DSSP) dataset
- 3 — Transfer free energy (Simon, 1976), Cited by Charton-Charton (1982)
- 4 — SWEIG index (Cornette et al., 1987)
- 5 — Weights for alpha-helix at the window position of -2 (Qian-Sejnowski, 1988)
- 6 — Normalized positional residue frequency at helix termini N3 (Aurora-Rose,
- 7 — Weights from the IFH scale (Jacobs-White, 1989)
- 8 — Modified Kyte-Doolittle hydrophobicity scale (Juretic et al., 1998)
- 9 — pK-N (Fasman, 1976)
- 10 — Normalized positional residue frequency at helix termini C'' (Aurora-Rose,
- 11 — Normalized frequency of extended structure (Burgess et al., 1974)
- 12 — Normalized positional residue frequency at helix termini N'' (Aurora-Rose,
- 13 — Weights for alpha-helix at the window position of -4 (Qian-Sejnowski, 1988)
- 14 — Weights for coil at the window position of -4 (Qian-Sejnowski, 1988)
- 15 — Normalized positional residue frequency at helix termini N1 (Aurora-Rose,
- 16 — Normalized positional residue frequency at helix termini N2 (Aurora-Rose,
- 17 — Distribution of amino acid residues in the alpha-helices in mesophilic
- 18 — Entire chain composition of amino acids in intracellular proteins of
- 19 — Membrane-buried preference parameters (Argos et al., 1982)
- 20 — Knowledge-based membrane-propensity scale from 1D.Helix in MPtopo databases
- 21 — Normalized frequency of beta-structure (Nagano, 1973)
- 22 — Normalized frequency of beta-sheet in all-beta class (Palau et al., 1981)
- 23 — Relative preference value at N4 (Richardson-Richardson, 1988)
- 24 — Mean area buried on transfer (Rose et al., 1985)
- 25 — Information measure for extended (Robson-Suzuki, 1976)
- 26 — Free energy in beta-strand conformation (Munoz-Serrano, 1994)
- 27 — Relative preference value at N2 (Richardson-Richardson, 1988)
- 28 — Relative preference value at N3 (Richardson-Richardson, 1988)
- 29 — Normalized frequency of beta-sheet in alpha+beta class (Palau et al., 1981)
- 30 — Average relative fractional occurrence in E0(i) (Rackovsky-Scheraga, 1982)
- 31 — Normalized frequency of coil (Tanaka-Scheraga, 1977)
- 32 — N.m.r. chemical shift of alpha-carbon (Fauchere et al., 1988)
- 33 — Weights for coil at the window position of 1 (Qian-Sejnowski, 1988)
- 34 — Weights for coil at the window position of 0 (Qian-Sejnowski, 1988)
- 35 — Weights for beta-sheet at the window position of -2 (Qian-Sejnowski, 1988)
- 36 — Relative preference value at C2 (Richardson-Richardson, 1988)
- 37 — Relative preference value at C1 (Richardson-Richardson, 1988)
- 38 — Hydrophobicity index (Fasman, 1989)
- 39 — Optimized relative partition energies - method C (Miyazawa-Jernigan, 1999)
- 40 — RF value in high salt chromatography (Weber-Lacey, 1978)
- 41 — Dependence of partition coefficient on ionic strength (Zaslavsky et al.,
- 42 — Normalized frequency of turn in all-alpha class (Palau et al., 1981)
- 43 — Normalized frequency of turn in alpha/beta class (Palau et al., 1981)
- 44 — Free energy in beta-strand region (Munoz-Serrano, 1994)
- 45 — Free energy in alpha-helical conformation (Munoz-Serrano, 1994)
- 46 — Positive charge (Fauchere et al., 1988)
- 47 — Entropy of formation (Hutchens, 1970)
- 48 — Weights for alpha-helix at the window position of -6 (Qian-Sejnowski, 1988)
- 49 — Hydrophobicity coefficient in RP-HPLC, C4 with 0.150 — A parameter of charge transfer donor capability (Charton-Charton, 1983)
- 51 — Composition of amino acids in extracellular proteins (percent) (Cedano et
- 52 — Weights for beta-sheet at the window position of 3 (Qian-Sejnowski, 1988)
- 53 — Average relative fractional occurrence in AR(i) (Rackovsky-Scheraga, 1982)
- 54 — Weights for coil at the window position of -3 (Qian-Sejnowski, 1988)
- 55 — Average relative fractional occurrence in EL(i) (Rackovsky-Scheraga, 1982)
- 56 — Heat capacity (Hutchens, 1970)
- 57 — Normalized frequency of turn in all-beta class (Palau et al., 1981)
- 58 — Hydrophobicity coefficient in RP-HPLC, C8 with 0.159 — Retention coefficient in HPLC, pH2.1 (Meek, 1980)
- 60 — Information measure for alpha-helix (Robson-Suzuki, 1976)
- 61 — Normalized frequency of alpha-helix in alpha/beta class (Palau et al., 1981)
- 62 — Side chain interaction parameter (Krigbaum-Rubin, 1971)
- 63 — Normalized frequency of N-terminal non helical region (Chou-Fasman, 1978b)
- 64 — Weights for beta-sheet at the window position of -5 (Qian-Sejnowski, 1988)
- 65 — Helix termination parameter at position j+1 (Finkelstein et al., 1991)
- 66 — Information measure for N-terminal helix (Robson-Suzuki, 1976)
- 67 — Normalized positional residue frequency at helix termini N'' (Aurora-Rose,
- 68 — Normalized frequency of alpha-helix in all-alpha class (Palau et al., 1981)
- 69 — Composition of amino acids in intracellular proteins (percent) (Cedano et
- 70 — AA composition of CYT of multi-spanning proteins (Nakashima-Nishikawa, 1992)
- 71 — Relative preference value at C5 (Richardson-Richardson, 1988)
- 72 — Normalized positional residue frequency at helix termini C'' (Aurora-Rose,
- 73 — Zimm-Bragg parameter sigma x 1.0E4 (Sueki et al., 1984)
- 74 — Weights for coil at the window position of -6 (Qian-Sejnowski, 1988)
- 75 — Normalized positional residue frequency at helix termini C2 (Aurora-Rose,
- 76 — Information measure for N-terminal turn (Robson-Suzuki, 1976)
- 77 — Transmembrane regions of mt-proteins (Nakashima et al., 1990)
- 78 — Interior composition of amino acids in nuclear proteins (percent)
- 79 — Weights for alpha-helix at the window position of 4 (Qian-Sejnowski, 1988)
- 80 — Information measure for C-terminal helix (Robson-Suzuki, 1976)
- 81 — Normalized positional residue frequency at helix termini C' (Aurora-Rose,
- 82 — Average relative fractional occurrence in AL(i-1) (Rackovsky-Scheraga, 1982)
- 83 — Beta-sheet propensity derived from designed sequences (Koehl-Levitt, 1999)
- 84 — Conformational preference for parallel beta-strands (Lifson-Sander, 1979)
- 85 — Principal property value z3 (Wold et al., 1987)
- 86 — Amphiphilicity index (Mitaku et al., 2002)
- 87 — Total weighted atomic number of the graph (obtained by summing all the atomic
- 88 — Second smallest eigenvalue of the Laplacian matrix of the graph
- 89 — Weighted second smallest eigenvalue of the weighted Laplacian matrix
- 90 — Relative preference value at C'' (Richardson-Richardson, 1988)
- 91 — Normalized frequency of isolated helix (Tanaka-Scheraga, 1977)
- 92 — Relative partition energies de-

rived by the Bethe approximation  
 93 — Buriability (Zhou-Zhou, 2004)  
 94 — Relative preference value at C3 (Richardson-Richardson, 1988)  
 95 — Alpha-helix propensity derived from designed sequences (Koehl-Levitt, 1999)  
 96 — Scaled side chain hydrophobicity values (Black-Mould, 1991)  
 97 — Hydrophobicity coefficient in RP-HPLC, C18 with 0.198 — Frequency of occurrence in beta-bends (Lewis et al., 1971)  
 99 — Normalized frequency of turn in alpha+beta class (Palau et al., 1981)  
 100 — Normalized flexibility parameters (B-values) for each residue surrounded by  
 101 — Apparent partition energies calculated from Janin index (Guy, 1985)  
 102 — Normalized frequency of alpha-helix in alpha+beta class (Palau et al., 1981)  
 103 — Weights for alpha-helix at the window position of -5 (Qian-Sejnowski, 1988)  
 104 — A parameter of charge transfer capability (Charton-Charton, 1983)  
 105 — Normalized frequency of extended structure (Tanaka-Scheraga, 1977)  
 106 — Normalized frequency of chain reversal S (Tanaka-Scheraga, 1977)  
 107 — Relative preference value at N-cap (Richardson-Richardson, 1988)  
 108 — Relative preference value at C' (Richardson-Richardson, 1988)  
 109 — Linker index (Bae et al., 2005)  
 110 — Weighted average eigenvalue based on the atomic numbers  
 111 — Maximum eigenvalue of the weighted Laplacian matrix of the graph  
 112 — Surrounding hydrophobicity in beta-sheet (Ponnuswamy et al., 1980)  
 113 — Average weighted eccentricity based on the the atomic number  
 114 — Principal property value z2 (Wold et al., 1987)  
 115 — Free energy of solution in water, kcal/mole (Charton-Charton, 1982)  
 116 — Linker propensity index (Suyama-Ohara, 2003)  
 117 — Normalized positional residue frequency at helix termini N4' (Aurora-Rose,  
 118 — Normalized positional residue frequency at helix termini C4' (Aurora-Rose,  
 119 — Activation Gibbs energy of unfolding, pH7.0 (Yutani et al., 1987)  
 120 — Apparent partition energies calculated from Chothia index (Guy, 1985)  
 121 — The Kerr-constant increments (Khanarian-Moore, 1980)  
 122 — Average weighted atomic number or degree based on atomic number in the graph  
 123 — Optimized average non-bonded energy per atom (Oobatake et al., 1985)  
 124 — Hydrophobicity coefficient in RP-HPLC, C18 with 0.1125 — Weights for coil at the window position of -5 (Qian-Sejnowski, 1988)  
 126 — Free energy change of epsilon(i) to epsilon(ex) (Wertz-Scheraga, 1978)  
 127 — Information measure for loop (Robson-Suzuki, 1976)  
 128 — Normalized positional residue frequency at helix termini Cc (Aurora-Rose,  
 129 — Ratio of average and computed composition (Nakashima et al., 1990)  
 130 — pK (-COOH) (Jones, 1975)  
 131 — Unfolding Gibbs energy in water, pH9.0 (Yutani et al., 1987)  
 132 — A parameter defined from the residuals obtained from the best correlation of  
 133 — Flexibility parameter for two rigid neighbors (Karplus-Schulz, 1985)  
 134 — Weights for beta-sheet at the window position of 6 (Qian-Sejnowski, 1988)  
 135 — Weights for beta-sheet at the window position of 5 (Qian-Sejnowski, 1988)  
 136 — Relative preference value at N1 (Richardson-Richardson, 1988)  
 137 — Loss of Side chain hydrophathy by helix formation (Roseman, 1988)  
 138 — Relative preference value at C4 (Richardson-Richardson, 1988)  
 139 — Average relative fractional occurrence in AL(i) (Rackovsky-Scheraga, 1982)  
 140 — Linker propensity from small dataset (linker length is less than six  
 141 — Relative population of conformational state E (Vasquez et al., 1983)  
 142 — Average relative fractional occurrence in A0(i-1) (Rackovsky-Scheraga, 1982)  
 143 — Linker propensity from helical (annotated by DSSP) dataset (George-Heringa,  
 144 — Average relative fractional occurrence in A0(i) (Rackovsky-Scheraga, 1982)  
 145 — Normalized frequency of chain reversal D (Tanaka-Scheraga, 1977)  
 146 — Polarity (Zimmerman et al., 1968)  
 147 — Principal component II (Sneath, 1966)  
 148 — Information measure for extended without H-bond (Robson-Suzuki, 1976)  
 149 — Weights for alpha-helix at the window position of 6 (Qian-Sejnowski, 1988)  
 150 — Principal component IV (Sneath, 1966)  
 151 — Normalized frequency of alpha region (Maxfield-Scheraga, 1976)  
 152 — Linker propensity from long dataset (linker length is greater than 14  
 153 — Partial specific volume (Cohn-Edsall, 1943)  
 154 — The number of atoms in the side chain labelled 1+1 (Charton-Charton, 1983)  
 155 — Weighted minimum eigenvalue based on the atomic numbers  
 156 — Normalized frequency of zeta R (Maxfield-Scheraga, 1976)  
 157 — Relative population of conformational state A (Vasquez et al., 1983)  
 158 — Free energy change of alpha(Ri) to alpha(Rh) (Wertz-Scheraga, 1978)  
 159 — Free energy change of epsilon(i) to alpha(Rh) (Wertz-Scheraga, 1978)  
 160 — Relative preference value at N' (Richardson-Richardson, 1988)  
 161 — Propensity of amino acids within pi-helices (Fodje-Al-Karadaghi, 2002)  
 162 — Hydropathy scale based on self-information values in the two-state model (50163 — Correlation coefficient in regression analysis (Prabhakaran-Ponnuswamy, 1982)  
 164 — Bulkiness (Zimmerman et al., 1968)  
 165 — Alpha-helix indices for beta-proteins (Geisow-Roberts, 1980)  
 166 — Weights for beta-sheet at the window position of -3 (Qian-Sejnowski, 1988)  
 167 — The number of atoms in the side chain labelled 2+1 (Charton-Charton, 1983)  
 168 — Principal component I (Sneath, 1966)  
 169 — Hydrostatic pressure asymmetry index, PAI (Di Giulio, 2005)  
 170 — Electron-ion interaction potential values (Cotic, 1994)  
 171 — alpha-CH chemical shifts (Bundi-Wuthrich, 1979)  
 172 — pK-a(RCOOH) (Fauchere et al., 1988)  
 173 — Normalized frequency of C-terminal non helical region (Chou-Fasman, 1978b)  
 174 — Surface composition of amino acids in intracellular proteins of mesophiles  
 175 — Normalized composition from fungi and plant (Nakashima et al., 1990)  
 176 — Hydrophobicity (Zimmerman et al., 1968)  
 177 — Thermodynamic beta sheet propensity (Kim-Berg, 1993)  
 178 — Melting point (Fasman, 1976)  
 179 — Relative mutability (Jones et al., 1992)  
 180 — Relative preference value at N5 (Richardson-Richardson, 1988)  
 181 — Net charge (Klein et al., 1984)  
 182 — Weights for coil at the window position of 5 (Qian-Sejnowski, 1988)  
 183 — Normalized relative frequency of double bend (Isogai et al., 1980)  
 184 — Composition (Grantham, 1974)  
 185 — Information measure for C-terminal turn (Robson-Suzuki, 1976)  
 186 — Linker propensity from medium dataset (linker length is between six and 14  
 187 — Weights for coil at the window position of 6 (Qian-Sejnowski, 1988)  
 188 — Normalized frequency of zeta R (Tanaka-Scheraga, 1977)  
 189 — Normalized positional residue frequency at helix termini N' (Aurora-Rose,  
 190 — Intercept in regression analysis (Prabhakaran-Ponnuswamy, 1982)  
 191 — Spin-spin coupling constants 3JHalpha-NH (Bundi-Wuthrich, 1979)