**Supplementary Materials**

**1. The 83 relative independently properties of AAindex1**

|  |  |  |
| --- | --- | --- |
| 1 | BUNA790103 | Spin-spin coupling constants 3JHalpha-NH (Bundi-Wuthrich, 1979) |
| 2 | QIAN880139 | Weights for coil at the window position of 6 (Qian-Sejnowski, 1988) |
| 3 | TANS770108 | Normalized frequency of zeta R (Tanaka-Scheraga, 1977) |
| 4 | VASM830101 | Relative population of conformational state A (Vasquez et al., 1983) |
| 5 | WERD780103 | Free energy change of alpha(Ri) to alpha(Rh) (Wertz-Scheraga, 1978) |
| 6 | MAXF760103 | Normalized frequency of zeta R (Maxfield-Scheraga, 1976) |
| 7 | RICJ880117 | Relative preference value at C" (Richardson-Richardson, 1988) |
| 8 | ROBB760107 | Information measure for extended without H-bond (Robson-Suzuki, 1976) |
| 9 | ROSM880103 | Loss of Side chain hydropathy by helix formation (Roseman, 1988) |
| 10 | WERD780102 | Free energy change of epsilon(i) to epsilon(ex) (Wertz-Scheraga, 1978) |
| 11 | WILM950104 | Hydrophobicity coefficient in RP-HPLC, C18 with 0.1%TFA/2-PrOH/MeCN/H2O (Wilce et al. 1995) |
| 12 | KHAG800101 | The Kerr-constant increments (Khanarian-Moore, 1980) |
| 13 | PRAM820103 | Correlation coefficient in regression analysis (Prabhakaran-Ponnuswamy, 1982) |
| 14 | QIAN880117 | Weights for beta-sheet at the window position of -3 (Qian-Sejnowski, 1988) |
| 15 | RACS820107 | Average relative fractional occurrence in A0(i-1) (Rackovsky-Scheraga, 1982) |
| 16 | VELV850101 | Electron-ion interaction potential (Veljkovic et al., 1985) |
| 17 | QIAN880123 | Weights for beta-sheet at the window position of 3 (Qian-Sejnowski, 1988) |
| 18 | RICJ880114 | Relative preference value at C1 (Richardson-Richardson, 1988) |
| 19 | SNEP660104 | Principal component IV (Sneath, 1966) |
| 20 | GEIM800103 | Alpha-helix indices for beta-proteins (Geisow-Roberts, 1980) |
| 21 | ISOY800107 | Normalized relative frequency of double bend (Isogai et al., 1980) |
| 22 | QIAN880128 | Weights for coil at the window position of -5 (Qian-Sejnowski, 1988) |
| 23 | ROBB760111 | Information measure for C-terminal turn (Robson-Suzuki, 1976) |
| 24 | AURR980118 | Normalized positional residue frequency at helix termini C" (Aurora-Rose, 1998) |
| 25 | AURR980120 | Normalized positional residue frequency at helix termini C4'' (Aurora-Rose, 1998) |
| 26 | NADH010107 | Hydropathy scale based on self-information values in the two-state model (50% accessibility) (Naderi-Manesh et al., 2001) |
| 27 | ISOY800106 | Normalized relative frequency of helix end (Isogai et al., 1980) |
| 28 | JOND920102 | Relative mutability (Jones et al., 1992) |
| 29 | PRAM820101 | Intercept in regression analysis (Prabhakaran-Ponnuswamy, 1982) |
| 30 | RICJ880101 | Relative preference value at N" (Richardson-Richardson, 1988) |
| 31 | RICJ880104 | Relative preference value at N1 (Richardson-Richardson, 1988) |
| 32 | SUEM840102 | Zimm-Bragg parameter sigma x 1.0E4 (Sueki et al., 1984) |
| 33 | VASM830102 | Relative population of conformational state C (Vasquez et al., 1983) |
| 34 | GEOR030103 | Linker propensity from 2-linker dataset (George-Heringa, 2003) |
| 35 | CHAM830102 | A parameter defined from the residuals obtained from the best correlation of the Chou-Fasman parameter of beta-sheet (Charton-Charton, 1983) |
| 36 | NAKH900113 | Ratio of average and computed composition (Nakashima et al., 1990) |
| 37 | RICJ880105 | Relative preference value at N2 (Richardson-Richardson, 1988) |
| 38 | WOLS870103 | Principal property value z3 (Wold et al., 1987) |
| 39 | GEOR030107 | Linker propensity from long dataset (linker length is greater than 14 residues) (George-Heringa, 2003) |
| 40 | QIAN880113 | Weights for alpha-helix at the window position of 6 (Qian-Sejnowski, 1988) |
| 41 | QIAN880129 | Weights for coil at the window position of -4 (Qian-Sejnowski, 1988) |
| 42 | RACS820103 | Average relative fractional occurrence in AL(i) (Rackovsky-Scheraga, 1982) |
| 43 | RACS820104 | Average relative fractional occurrence in EL(i) (Rackovsky-Scheraga, 1982)' |
| 44 | FASG760104 | pK-N (Fasman, 1976) |
| 45 | JOND750102 | pK (-COOH) (Jones, 1975) |
| 46 | KLEP840101 | Net charge (Klein et al., 1984) |
| 47 | FAUJ880108 | Localized electrical effect (Fauchere et al., 1988) |
| 48 | RICJ880108 | Relative preference value at N5 (Richardson-Richardson, 1988) |
| 49 | CHOP780206 | Normalized frequency of N-terminal non helical region (Chou-Fasman, 1978b) |
| 50 | BUNA790102 | alpha-CH chemical shifts (Bundi-Wuthrich, 1979) |
| 51 | OOBM850104 | Optimized average non-bonded energy per atom (Oobatake et al., 1985) |
| 52 | FASG760103 | Optical rotation (Fasman, 1976) |
| 53 | AVBF000106 | Slopes tripeptide FDPB VFF all (Avbelj, 2000) |
| 54 | QIAN880102 | Weights for alpha-helix at the window position of -5 (Qian-Sejnowski, 1988) |
| 55 | RACS820106 | Average relative fractional occurrence in ER(i) (Rackovsky-Scheraga, 1982) |
| 56 | AURR980105 | Normalized positional residue frequency at helix termini Nc (Aurora-Rose, 1998) |
| 57 | DIGM050101 | Hydrostatic pressure asymmetry index, PAI (Di Giulio, 2005) |
| 58 | KARP850103 | Flexibility parameter for two rigid neighbors (Karplus-Schulz, 1985) |
| 59 | NAKH900105 | AA composition of mt-proteins from animal (Nakashima et al., 1990) |
| 60 | CHOP780207 | Normalized frequency of C-terminal non helical region (Chou-Fasman, 1978b) |
| 61 | AURR980116 | Normalized positional residue frequency at helix termini Cc (Aurora-Rose, 1998) |
| 62 | BURA740102 | Normalized frequency of extended structure (Burgess et al., 1974) |
| 63 | SNEP660102 | Principal component II (Sneath, 1966) |
| 64 | CHAM830103 | The number of atoms in the side chain labelled 1+1 (Charton-Charton, 1983) |
| 65 | RACS820101 | Average relative fractional occurrence in A0(i) (Rackovsky-Scheraga, 1982) |
| 66 | NAKH920104 | AA composition of EXT2 of single-spanning proteins (Nakashima-Nishikawa, 1992) |
| 67 | SNEP660101 | Principal component I (Sneath, 1966) |
| 68 | RICJ880116 | Relative preference value at C'' (Richardson-Richardson, 1988) |
| 69 | MITS020101 | Amphiphilicity index (Mitaku et al., 2002) |
| 70 | KUMS000103 | Distribution of amino acid residues in the alpha-helices in thermophilic proteins (Kumar et al., 2000) |
| 71 | HUTJ700103 | Entropy of formation (Hutchens, 1970) |
| 72 | ZIMJ680101 | Hydrophobicity (Zimmerman et al., 1968) |
| 73 | RICJ880112 | Relative preference value at C3 (Richardson-Richardson, 1988) |
| 74 | NAKH900108 | Normalized composition from fungi and plant (Nakashima et al., 1990) |
| 75 | PALJ810116 | Normalized frequency of turn in alpha/beta class (Palau et al., 1981) |
| 76 | ZIMJ680103 | Polarity (Zimmerman et al., 1968) |
| 77 | PALJ810115 | Normalized frequency of turn in alpha+beta class (Palau et al., 1981) |
| 78 | GEOR030105 | Linker propensity from small dataset (linker length is less than six residues) (George-Heringa, 2003) |
| 79 | QIAN880118 | Weights for beta-sheet at the window position of -2 (Qian-Sejnowski, 1988) |
| 80 | AURR980113 | Normalized positional residue frequency at helix termini C3 (Aurora-Rose, 1998) |
| 81 | PONP800105 | Surrounding hydrophobicity in beta-sheet (Ponnuswamy et al., 1980)' |
| 82 | WILM950102 | Hydrophobicity coefficient in RP-HPLC, C8 with 0.1%TFA/MeCN/H2O (Wilce et al. 1995) |
| 83 | ROSG850101 | Mean area buried on transfer (Rose et al., 1985) |

**2. The 23 properties in the combination of top 23 classifiers based-on ASEdb**

The feature number ranked in descend sort according to F1 score:

62, 16, 26, 10, 5, 44, 70, 21, 12, 41, 53, 32, 6, 57, 40, 82,79, 39, 29, 71, 30, 58, 13

**3. The 13 properties in the combination of top 13 classifiers based-on SKEMPI**

The feature number ranked in descend sort according to F1 score:

28, 61, 34, 26, 32, 65, 68, 42, 35, 59, 4, 44, 57

**4. Table S1 Training dataset respectively on ASEdb1 , ASEdb2 and ASEdb3 dataset**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **PDB\_ID** | **Residue** | **Chain** | **Robetta** | **ΔΔGobs** | **Observed on ASEdb1** | **Observed on ASEdb2** | **Observed on ASEdb3** |
| 1A4Y | W261 | A | 1.06 | 0.1 | -- | -- | -- |
| 1A4Y | W263 | A | 2.27 | 1.2 | / | -- | \*\* |
| 1A4Y | S289 | A | 0.6 | 0 | -- | -- | -- |
| 1A4Y | W318 | A | 2.19 | 1.5 | / | -- | \*\* |
| 1A4Y | K320 | A | -0.21 | -0.3 | -- | -- | -- |
| 1A4Y | E344 | A | 1.37 | 0.2 | -- | -- | -- |
| 1A4Y | W375 | A | 2.83 | 1 | / | -- | \*\* |
| 1A4Y | E401 | A | 0.02 | 0.9 | / | -- | -- |
| 1A4Y | Y434 | A | 3 | 3.3 | \*\* | \*\* | \*\* |
| 1A4Y | D435 | A | 0.58 | 3.5 | \*\* | \*\* | \*\* |
| 1A4Y | Y437 | A | 3.13 | 0.8 | / | -- | -- |
| 1A4Y | I459 | A | 0.62 | 0.7 | / | -- | -- |
| 1A4Y | R5 | B | 2.54 | 2.3 | \*\* | \*\* | \*\* |
| 1A4Y | H8 | B | 0.85 | 0.9 | / | -- | -- |
| 1A4Y | Q12 | B | 0.87 | 0.3 | -- | -- | -- |
| 1A4Y | R31 | B | 2.76 | 0.2 | -- | -- | -- |
| 1A4Y | R32 | B | 0.18 | 0.9 | / | -- | -- |
| 1A4Y | N68 | B | 0.52 | 0.2 | -- | -- | -- |
| 1A4Y | H84 | B | 1.05 | 0.2 | -- | -- | -- |
| 1A4Y | W89 | B | 2.71 | 0.2 | -- | -- | -- |
| 1A4Y | E108 | B | 1.73 | -0.3 | -- | -- | -- |
| 1A4Y | H114 | B | 1.69 | 0.65 | / | -- | -- |
| 1AHW | Y156 | C | 4.53 | 4 | \*\* | \*\* | \*\* |
| 1AHW | T167 | C | -0.24 | 0 | -- | -- | -- |
| 1AHW | T170 | C | -0.06 | 1 | / | -- | \*\* |
| 1AHW | V198 | C | -0.01 | -0.3 | -- | -- | -- |
| 1BRS | K27 | A | 1.88 | 5.4 | \*\* | \*\* | \*\* |
| 1BRS | N58 | A | -0.03 | 3.1 | \*\* | \*\* | \*\* |
| 1BRS | R59 | A | 3.01 | 5.2 | \*\* | \*\* | \*\* |
| 1BRS | E60 | A | 1.41 | -0.2 | -- | -- | -- |
| 1BRS | R83 | A | 6.84 | 5.4 | \*\* | \*\* | \*\* |
| 1BRS | R87 | A | 4.44 | 5.5 | \*\* | \*\* | \*\* |
| 1BRS | H102 | A | 5.08 | 6.1 | \*\* | \*\* | \*\* |
| 1BRS | Y29 | D | 3.13 | 3.4 | \*\* | \*\* | \*\* |
| 1BRS | D35 | D | 1.42 | 4.5 | \*\* | \*\* | \*\* |
| 1BRS | D39 | D | 9.4 | 7.7 | \*\* | \*\* | \*\* |
| 1BRS | T42 | D | 1.66 | 1.8 | / | -- | \*\* |
| 1BRS | E76 | D | 1.54 | 1.3 | / | -- | \*\* |
| 1BXI | C23 | A | -0.08 | 0.92 | / | -- | -- |
| 1BXI | N24 | A | 0 | 0.14 | -- | -- | -- |
| 1BXI | T27 | A | 0.59 | 0.73 | / | -- | -- |
| 1BXI | S28 | A | 0 | 0.17 | -- | -- | -- |
| 1BXI | S29 | A | 0.17 | 0.96 | / | -- | -- |
| 1BXI | E30 | A | 2.97 | 1.41 | / | -- | \*\* |
| 1BXI | L33 | A | 1.02 | 3.42 | \*\* | \*\* | \*\* |
| 1BXI | V34 | A | 0.98 | 2.58 | \*\* | \*\* | \*\* |
| 1BXI | V37 | A | 0.5 | 1.66 | / | -- | \*\* |
| 1BXI | T38 | A | 1.35 | 0.9 | / | -- | -- |
| 1BXI | E41 | A | -0.07 | 2.08 | \*\* | \*\* | \*\* |
| 1BXI | S48 | A | -0.01 | 0.01 | -- | -- | -- |
| 1BXI | S50 | A | 4.21 | 2.19 | \*\* | \*\* | \*\* |
| 1BXI | D51 | A | 0.82 | 5.92 | \*\* | \*\* | \*\* |
| 1BXI | I53 | A | 0.17 | 0.85 | / | -- | -- |
| 1BXI | Y54 | A | 2.85 | 4.83 | \*\* | \*\* | \*\* |
| 1BXI | Y55 | A | 3.49 | 4.63 | \*\* | \*\* | \*\* |
| 1CBW | T11 | D | 0.18 | 0.2 | -- | -- | -- |
| 1CBW | K15 | D | 1.58 | 2 | \*\* | \*\* | \*\* |
| 1CBW | R17 | D | 1.53 | 0.5 | / | -- | -- |
| 1CBW | R39 | D | 1.58 | 0.2 | -- | -- | -- |
| 1DAN | L39 | L | 1.24 | 0 | -- | -- | -- |
| 1DAN | K62 | L | -0.27 | 0 | -- | -- | -- |
| 1DAN | Q64 | L | 2.98 | 0.8 | / | -- | -- |
| 1DAN | I69 | L | 1.57 | 1.9 | / | -- | \*\* |
| 1DAN | F71 | L | 3.07 | 1.2 | / | -- | \*\* |
| 1DAN | L73 | L | 0 | 0 | -- | -- | -- |
| 1DAN | E77 | L | 0.36 | 0 | -- | -- | -- |
| 1DAN | R79 | L | 2.45 | 1.2 | / | -- | \*\* |
| 1DAN | Q88 | L | 0.35 | 0 | -- | -- | -- |
| 1DAN | V92 | L | 0.09 | 0 | -- | -- | -- |
| 1DAN | N93 | L | 0.12 | 0 | -- | -- | -- |
| 1DAN | E94 | L | -0.1 | 0 | -- | -- | -- |
| 1DAN | H115 | L | 0.93 | 0 | -- | -- | -- |
| 1DAN | T17 | T | 0.12 | 0.1 | -- | -- | -- |
| 1DAN | K20 | T | 1.5 | 2.6 | \*\* | \*\* | \*\* |
| 1DAN | I22 | T | 0.65 | 0.7 | / | -- | -- |
| 1DAN | E24 | T | 0.64 | 0.7 | / | -- | -- |
| 1DAN | Q37 | T | 1.4 | 0.55 | / | -- | -- |
| 1DAN | K41 | T | -0.04 | 0.35 | -- | -- | -- |
| 1DAN | S42 | T | -0.05 | -0.1 | -- | -- | -- |
| 1DAN | D44 | T | 0.9 | 0.7 | / | -- | -- |
| 1DAN | W45 | T | 1.05 | 1.6 | / | -- | \*\* |
| 1DAN | S47 | T | -0.05 | 0.05 | -- | -- | -- |
| 1DAN | K48 | T | 0.43 | 0.4 | / | -- | -- |
| 1DAN | F50 | T | 2.61 | 0.4 | / | -- | -- |
| 1DAN | D58 | T | 1.09 | 2.18 | \*\* | \*\* | \*\* |
| 1DAN | D61 | T | 0.01 | 0.24 | -- | -- | -- |
| 1DAN | F76 | T | 0.61 | 1.2 | / | -- | \*\* |
| 1DAN | Y94 | U | 2.7 | 1 | / | -- | \*\* |
| 1DAN | Q110 | U | 1.69 | 1.4 | / | -- | \*\* |
| 1DAN | E128 | U | -0.11 | 0.1 | -- | -- | -- |
| 1DAN | R131 | U | 0.28 | 0 | -- | -- | -- |
| 1DAN | T132 | U | 0 | 0 | -- | -- | -- |
| 1DAN | L133 | U | 1.62 | 0 | -- | -- | -- |
| 1DAN | R135 | U | 0.94 | 0.55 | / | -- | -- |
| 1DAN | F140 | U | 1.54 | 1.5 | / | -- | \*\* |
| 1DAN | S163 | U | 0.42 | 0 | -- | -- | -- |
| 1DAN | T203 | U | 0.22 | 0.1 | -- | -- | -- |
| 1DAN | V207 | U | 1.12 | -0.2 | -- | -- | -- |
| 1DAN | E208 | U | 0.28 | 0 | -- | -- | -- |
| 1DVF | H30 | A | 0.26 | 1.7 | / | -- | \*\* |
| 1DVF | Y32 | A | 0.47 | 2 | \*\* | \*\* | \*\* |
| 1DVF | Y49 | A | 0.88 | 1.7 | / | -- | \*\* |
| 1DVF | Y50 | A | 0.58 | 0.7 | / | -- | -- |
| 1DVF | W92 | A | 1.56 | 0.3 | -- | -- | -- |
| 1DVF | T30 | B | 0.01 | 0.9 | / | -- | -- |
| 1DVF | Y32 | B | 0.11 | 1.8 | / | -- | \*\* |
| 1DVF | W52 | B | 3.26 | 4.2 | \*\* | \*\* | \*\* |
| 1DVF | D54 | B | 0.72 | 4.3 | \*\* | \*\* | \*\* |
| 1DVF | N56 | B | 1.07 | 1.2 | / | -- | \*\* |
| 1DVF | D58 | B | 0.71 | 1.6 | / | -- | \*\* |
| 1DVF | E98 | B | 0.05 | 4.2 | \*\* | \*\* | \*\* |
| 1DVF | R99 | B | 0.22 | 1.9 | / | -- | \*\* |
| 1DVF | D100 | B | 0.43 | 2.8 | \*\* | \*\* | \*\* |
| 1DVF | Y101 | B | 2.13 | 4 | \*\* | \*\* | \*\* |
| 1DVF | K30 | D | -0.04 | 0.9 | / | -- | -- |
| 1DVF | H33 | D | 0.79 | 1.9 | / | -- | \*\* |
| 1DVF | I97 | D | 1.07 | 2.7 | \*\* | \*\* | \*\* |
| 1DVF | Y98 | D | 4.78 | 4.7 | \*\* | \*\* | \*\* |
| 1DVF | Q100 | D | 1.44 | 1.6 | / | -- | \*\* |
| 1DX5 | F34 | M | 1.01 | 2.6 | \*\* | \*\* | \*\* |
| 1DX5 | Q38 | M | 2.31 | 1.4 | / | -- | \*\* |
| 1DX5 | R67 | M | -0.01 | 3.4 | \*\* | \*\* | \*\* |
| 1DX5 | T74 | M | 0.2 | 0.8 | / | -- | -- |
| 1DX5 | R75 | M | 0.05 | 0.7 | / | - | -- |
| 1DX5 | Y76 | M | 2.03 | 3 | \*\* | \*\* | \*\* |
| 1DX5 | K81 | M | 0.8 | 1 | / | -- | \*\* |
| 1DX5 | I82 | M | 1.07 | 2.6 | \*\* | \*\* | \*\* |
| 1DX5 | M84 | M | 0.77 | 0.3 | -- | -- | -- |
| 1DX5 | K110 | M | 0.17 | 0 | -- | -- | -- |
| 1GC1 | Q25 | C | 0.42 | 0.03 | -- | -- | -- |
| 1GC1 | H27 | C | 0.8 | 0.28 | -- | -- | -- |
| 1GC1 | K29 | C | 2.46 | 0.59 | / | -- | -- |
| 1GC1 | N32 | C | 0 | 0.18 | -- | -- | -- |
| 1GC1 | Q33 | C | 0.03 | 0.1 | -- | -- | -- |
| 1GC1 | K35 | C | 0.55 | 0.32 | -- | -- | -- |
| 1GC1 | Q40 | C | 1.66 | -0.41 | -- | -- | -- |
| 1GC1 | S42 | C | 0.03 | 0 | -- | -- | -- |
| 1GC1 | L44 | C | 0.07 | 1.04 | / | -- | \*\* |
| 1GC1 | T45 | C | 0.32 | -0.15 | -- | -- | -- |
| 1GC1 | N52 | C | 1.01 | 0.7 | / | -- | -- |
| 1GC1 | R59 | C | 1.02 | 1.16 | / | -- | \*\* |
| 1GC1 | S60 | C | 0.14 | -0.09 | -- | -- | -- |
| 1GC1 | D63 | C | -0.05 | -0.32 | -- | -- | -- |
| 1GC1 | Q64 | C | 1.02 | 0.44 | / | -- | -- |
| 1JTG | E104 | A | 2.1 | 1.55 | / | -- | \*\* |
| 1JTG | Y105 | A | 4.49 | -0.17 | -- | -- | -- |
| 1JTG | S130 | A | -0.18 | 0.8 | / | -- | -- |
| 1JTG | K234 | A | 0.6 | 1.4 | / | -- | \*\* |
| 1JTG | S235 | A | 2.33 | 1.3 | / | -- | \*\* |
| 1JTG | R243 | A | 3.76 | 1.4 | / | -- | \*\* |
| 1JTG | D49 | B | 6.42 | 1.8 | / | -- | \*\* |
| 1JTG | K74 | B | 0.68 | 3.56 | \*\* | \*\* | \*\* |
| 1JTG | F142 | B | 3.23 | 2.1 | \*\* | \*\* | \*\* |
| 1JTG | Y143 | B | 0.83 | 0.38 | -- | -- | -- |
| 1NMB | D56 | H | 3.64 | 2.8 | \*\* | \*\* | \*\* |
| 1NMB | Y99 | H | 1.28 | 1.5 | / | -- | \*\* |
| 1NMB | Y100 | H | 0.08 | 0.5 | / | -- | -- |
| 1NMB | Y32 | L | 2.19 | 1.7 | / | -- | \*\* |
| 1NMB | T93 | L | 1.41 | 0.3 | -- | -- | -- |
| 1NMB | L94 | L | 0.51 | 0.9 | / | -- | -- |
| 1VFB | W52 | B | 0.23 | 1.23 | / | -- | \*\* |
| 1VFB | D58 | B | 0.27 | -0.2 | -- | -- | -- |
| 1VFB | E98 | B | 4.79 | 1.1 | / | -- | \*\* |
| 1VFB | Y101 | B | 1.17 | 4 | \*\* | \*\* | \*\* |
| 3HFM | S31 | H | 0.38 | 0.2 | -- | -- | -- |
| 3HFM | D32 | H | 1.1 | 2 | \*\* | \*\* | \*\* |
| 3HFM | Y33 | H | 2.9 | 6 | \*\* | \*\* | \*\* |
| 3HFM | Y50 | H | 2.96 | 7.5 | \*\* | \*\* | \*\* |
| 3HFM | Y53 | H | 1.66 | 3.29 | \*\* | \*\* | \*\* |
| 3HFM | Y58 | H | 1.77 | 1.7 | / | -- | \*\* |
| 3HFM | N31 | L | 1.86 | 5.25 | \*\* | \*\* | \*\* |
| 3HFM | N32 | L | 2.48 | 5.2 | \*\* | \*\* | \*\* |
| 3HFM | Y50 | L | 1.4 | 4.6 | \*\* | \*\* | \*\* |
| 3HFM | Q53 | L | 0.83 | 1 | / | -- | \*\* |
| 3HFM | Y96 | L | 0.45 | 2.8 | \*\* | \*\* | \*\* |
| 3HFM | H15 | Y | 0.09 | -0.44 | -- | -- | -- |
| 3HFM | Y20 | Y | 2.23 | 5 | -- | \*\* | \*\* |
| 3HFM | R21 | Y | 3.42 | 1 | / | -- | \*\* |
| 3HFM | W63 | Y | 0.83 | 0.31 | -- | -- | -- |
| 3HFM | R73 | Y | 0.62 | -0.2 | -- | -- | -- |
| 3HFM | L75 | Y | 1.31 | 1.25 | / | -- | \*\* |
| 3HFM | T89 | Y | 0.17 | 0 | -- | -- | -- |
| 3HFM | N93 | Y | 1.53 | 0.6 | / | -- | -- |
| 3HFM | K96 | Y | 2.13 | 7 | \*\* | \*\* | \*\* |
| 3HFM | K97 | Y | 1.42 | 6 | \*\* | \*\* | \*\* |
| 3HFM | I98 | Y | 0.1 | 0 | -- | -- | -- |
| 3HFM | S100 | Y | 0.84 | 0.26 | -- | -- | -- |
| 3HFM | D101 | Y | 0.32 | 0.94 | / | -- | -- |
| 3HHR | I4 | A | 1.05 | 0.41 | / | -- | -- |
| 3HHR | R8 | A | 1.36 | 0.2 | -- | -- | -- |
| 3HHR | L9 | A | 0.44 | -0.04 | -- | -- | -- |
| 3HHR | N12 | A | 3.02 | 0.1 | -- | -- | -- |
| 3HHR | L15 | A | 1.27 | 0.15 | -- | -- | -- |
| 3HHR | R16 | A | 2.78 | 0.24 | -- | -- | -- |
| 3HHR | H18 | A | 1.51 | -0.5 | -- | -- | -- |
| 3HHR | H21 | A | 0.64 | 0.2 | -- | -- | -- |
| 3HHR | Q22 | A | 0.06 | -0.2 | -- | -- | -- |
| 3HHR | F25 | A | 1.68 | -0.4 | -- | -- | -- |
| 3HHR | Y42 | A | 2.09 | 0.2 | -- | -- | -- |
| 3HHR | L45 | A | 1.15 | 1.2 | / | -- | \*\* |
| 3HHR | Q46 | A | 1.2 | 0.1 | -- | -- | -- |
| 3HHR | S62 | A | 0.18 | 0.2 | -- | -- | -- |
| 3HHR | N63 | A | 0.22 | 0.3 | -- | -- | -- |
| 3HHR | R64 | A | 1.12 | 1.6 | / | -- | \*\* |
| 3HHR | Q68 | A | 0.29 | 0.6 | / | -- | -- |
| 3HHR | Y164 | A | 0.6 | 0.3 | -- | -- | -- |
| 3HHR | R167 | A | 0.54 | 0.3 | -- | -- | -- |
| 3HHR | K168 | A | 1.14 | -0.2 | -- | -- | -- |
| 3HHR | D171 | A | 1.4 | 0.8 | / | -- | -- |
| 3HHR | K172 | A | 0.71 | 2 | / | \*\* | \*\* |
| 3HHR | E174 | A | 0.61 | -0.9 | -- | -- | -- |
| 3HHR | T175 | A | 2.86 | 2 | \*\* | \*\* | \*\* |
| 3HHR | R178 | A | 0.85 | 2.4 | \*\* | \*\* | \*\* |
| 3HHR | I179 | A | 1.06 | 0.8 | / | -- | -- |
| 3HHR | C182 | A | -0.1 | 1.01 | / | -- | \*\* |
| 3HHR | R43 | B | 3.18 | 2.2 | \*\* | \*\* | \*\* |
| 3HHR | E44 | B | 0.05 | 1.8 | / | -- | \*\* |
| 3HHR | W76 | B | 2 | 0.6 | / | -- | -- |
| 3HHR | T77 | B | 0.93 | -0.25 | -- | -- | -- |
| 3HHR | S102 | B | 0.33 | -0.2 | -- | -- | -- |
| 3HHR | I103 | B | 0.42 | 1.8 | / | -- | \*\* |
| 3HHR | W104 | B | 4.98 | 4.5 | \*\* | \*\* | \*\* |
| 3HHR | I105 | B | 0.15 | 2 | \*\* | \*\* | \*\* |
| 3HHR | C108 | B | -0.04 | 0 | -- | -- | -- |
| 3HHR | E120 | B | 0.59 | -0.2 | -- | -- | -- |
| 3HHR | K121 | B | 0.09 | 0.1 | -- | -- | -- |
| 3HHR | C122 | B | -0.2 | 0 | -- | -- | -- |
| 3HHR | D126 | B | -0.04 | 1 | / | -- | \*\* |
| 3HHR | E127 | B | 1.13 | 1 | / | -- | \*\* |
| 3HHR | D164 | B | 0.37 | 1.6 | / | -- | \*\* |
| 3HHR | I165 | B | 0.06 | 2.2 | \*\* | \*\* | \*\* |
| 3HHR | Q166 | B | 0.42 | 0 | -- | -- | -- |
| 3HHR | K167 | B | 0.02 | 0 | -- | -- | -- |
| 3HHR | W169 | B | 3.47 | 4.5 | \*\* | \*\* | \*\* |
| 3HHR | R217 | B | 0.17 | 0.2 | -- | -- | -- |
| 3HHR | N218 | B | 1.48 | 0.3 | -- | -- | -- |

\*\* represents hotspot

-- represents non-hotspot

/ represents the residue not included

**5. Table S2& Test dataset derived from BID**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **PDB\_ID** | **Residue** | **Chain** | **CompASA** | **Potential** | **DiffASA** | **Cons.** | **Robetta** | **Strength1** |
| 1CDL | F12 | A | 12.10 | 24.99 | 13.30 | 5 | 0.7 | W |
| 1CDL | F19 | A | 0.27 | 43.94 | 23.36 | 7 | 1.79 | W |
| 1CDL | F92 | A | 0.44 | 58.79 | 19.82 | 8 | 1.51 | S |
| 1CDL | K799 | E | 34.69 | 8.90 | 46.15 | 1 | 0.61 | N |
| 1CDL | W800 | E | 0.74 | 49.76 | 73.62 | 6 | 5.18 | S |
| 1CDL | K802 | E | 17.65 | 6.07 | 53.93 | 8 | 1.53 | I |
| 1CDL | R808 | E | 14.26 | 27.80 | 36.96 | 4 | 2.7 | I |
| 1CDL | I810 | E | 5.33 | 48.01 | 59.56 | 1 | 1.9 | S |
| 1CDL | L813 | E | 3.96 | 44.03 | 81.08 | 1 | 2.01 | S |
| 1DDM | I144 | A | 0.67 | 48.58 | 8.66 | 8 | 0.2 | S |
| 1DDM | E145 | A | 27.20 | 10.79 | 47.64 | 5 | 0.05 | S |
| 1DDM | K146 | A | 40.14 | 5.53 | 25.19 | 7 | 0.19 | I |
| 1DDM | S148 | A | 14.07 | 11.80 | 15.77 | 9 | 0 | N |
| 1DDM | C150 | A | 7.09 | 27.76 | 32.66 | 6 | -0.06 | S |
| 1DDM | R165 | A | 28.21 | 9.48 | 23.04 | 7 | 0.46 | I |
| 1DDM | C198 | A | 23.47 | 22.38 | 13.41 | 6 | -0.08 | S |
| 1DDM | F2 | B | 26.82 | 21.37 | 72.11 | 7 | 3.01 | I |
| 1DDM | S3 | B | 39.26 | 4.01 | 43.97 | 9 | -0.18 | S |
| 1DDM | N4 | B | 3.39 | 4.52 | 69.88 | 1 | 1.71 | S |
| 1DDM | M5 | B | 64.65 | 11.82 | 20.36 | 8 | 0.19 | S |
| 1DDM | S6 | B | 20.61 | 10.10 | 73.41 | 5 | 0.41 | S |
| 1DDM | F7 | B | 41.25 | 0.00 | 10.93 | 4 | 0.19 | S |
| 1DDM | E8 | B | 57.18 | 5.68 | 25.46 | 6 | 0.13 | W |
| 1DDM | F10 | B | 24.52 | 11.27 | 55.77 | 1 | 1.67 | W |
| 1DFJ | K7 | E | 31.23 | 10.13 | 18.58 | 4 | 0.26 | S |
| 1DVA | L32 | H | 0.06 | 48.73 | 2.24 | 8 | 0.41 | S |
| 1DVA | L34 | H | 0.18 | 34.32 | 15.97 | 6 | 1.25 | S |
| 1DVA | N37 | H | 41.34 | 1.99 | 20.89 | 2 | 0.01 | N |
| 1DVA | I65 | H | 6.60 | 10.40 | 14.68 | 2 | 0.73 | N |
| 1DVA | V67 | H | 0.15 | 35.61 | 15.43 | 5 | 0.7 | N |
| 1DVA | E70 | H | 7.77 | 22.00 | 4.66 | 5 | 1.02 | W |
| 1DVA | L73 | H | 0.48 | 52.77 | 32.97 | 4 | 0.53 | N |
| 1DVA | S74 | H | 41.88 | 6.69 | 25.56 | 2 | 0.11 | N |
| 1DVA | E75 | H | 59.15 | 0.00 | 6.15 | 2 | 0 | N |
| 1DVA | H76 | H | 46.23 | 13.73 | 32.60 | 1 | 0.43 | S |
| 1DVA | E80 | H | 10.37 | 16.60 | 12.85 | 5 | 0.01 | N |
| 1DVA | S82 | H | 29.70 | 12.88 | 33.24 | 2 | -0.01 | N |
| 1DVA | L144 | H | 4.83 | 34.00 | 11.76 | 6 | 0.28 | N |
| 1DVA | L153 | H | 6.19 | 37.80 | 23.92 | 2 | 0.82 | W |
| 1DVA | L2 | X | 8.35 | 54.51 | 54.82 | 5 | 2.31 | S |
| 1DVA | R7 | X | 32.84 | 10.98 | 58.81 | 6 | 4.4 | W |
| 1DVA | V8 | X | 7.23 | 22.63 | 15.43 | 1 | 0.57 | I |
| 1DVA | D9 | X | 9.98 | 7.63 | 51.02 | 5 | 0.66 | I |
| 1DVA | W11 | X | 19.37 | 25.46 | 36.65 | 5 | 2.61 | S |
| 1DVA | Y12 | X | 0.01 | 35.38 | 41.99 | 9 | 3.16 | S |
| 1DVA | F15 | X | 12.46 | 31.58 | 47.84 | 5 | 1.58 | S |
| 1DZI | N154 | A | 23.50 | 11.21 | 47.74 | 6 | 0.22 | I |
| 1DZI | Y157 | A | 59.56 | 5.67 | 1.65 | 7 | 1.5 | S |
| 1DZI | Q215 | A | 18.05 | 9.76 | 17.69 | 6 | 0.37 | S |
| 1DZI | D219 | A | 34.93 | 6.42 | 45.39 | 4 | 3.33 | I |
| 1DZI | L220 | A | 20.18 | 13.80 | 19.86 | 5 | 0.81 | N |
| 1DZI | T221 | A | 0.04 | 24.78 | 3.21 | 9 | 0.15 | S |
| 1DZI | E256 | A | 44.68 | 16.16 | 2.36 | 7 | 0.05 | N |
| 1DZI | H258 | A | 30.55 | 18.05 | 30.35 | 8 | 2.56 | I |
| 1EBP | F93 | A | 55.43 | 26.52 | 14.57 | 7 | 0.75 | S |
| 1EBP | M150 | A | 0.28 | 23.00 | 49.61 | 7 | 1.56 | S |
| 1EBP | T151 | A | 16.83 | 8.57 | 22.45 | 2 | -0.03 | W |
| 1EBP | F205 | A | 1.45 | 53.48 | 5.25 | 6 | 0.71 | S |
| 1EBP | L11 | C | 60.59 | 8.40 | 34.30 | 7 | 0.49 | N |
| 1EBP | T12 | C | 43.05 | 8.28 | 25.30 | 1 | -0.24 | I |
| 1EBP | W13 | C | 38.52 | 34.71 | 21.46 | 1 | 1.29 | S |
| 1ES7 | F49 | A | 7.71 | 35.80 | 54.13 | 2 | 2.78 | I |
| 1FCC | E27 | C | 0.81 | 21.09 | 34.61 | 8 | 3.14 | S |
| 1FCC | K28 | C | 5.78 | 14.09 | 70.46 | 1 | 0.99 | W |
| 1FCC | K31 | C | 1.58 | 18.33 | 36.66 | 1 | 1.91 | S |
| 1FCC | N35 | C | 22.38 | 9.59 | 55.88 | 9 | 1.18 | I |
| 1FCC | D40 | C | 50.25 | 7.35 | 29.25 | 1 | -0.15 | N |
| 1FCC | E42 | C | 56.07 | 5.80 | 22.55 | 1 | 0.03 | N |
| 1FCC | W43 | C | 4.07 | 31.82 | 22.27 | 6 | 2.71 | S |
| 1FOE | S41 | B | 13.67 | 16.76 | 50.00 | 6 | 2.11 | I |
| 1GL4 | R403 | A | 18.56 | 16.65 | 32.33 | 9 | 1.57 | I |
| 1GL4 | D427 | A | 15.71 | 14.89 | 35.91 | 7 | 0.77 | S |
| 1GL4 | H429 | A | 1.34 | 21.77 | 42.34 | 8 | 6.79 | S |
| 1GL4 | Y431 | A | 2.13 | 22.56 | 42.00 | 6 | 1.72 | S |
| 1GL4 | Y440 | A | 7.84 | 12.13 | 43.52 | 7 | 3.32 | I |
| 1GL4 | E616 | A | 55.76 | 7.67 | 15.22 | 7 | 0.91 | S |
| 1GL4 | R620 | A | 8.83 | 24.32 | 35.84 | 9 | 2.07 | S |
| 1JAT | E55 | A | 2.75 | 22.90 | 16.45 | 1 | 2.39 | S |
| 1JAT | F8 | B | 1.56 | 19.27 | 60.67 | 9 | 4.45 | S |
| 1K4U | R368 | P | 39.41 | 16.39 | 34.44 | 9 | 0.38 | S |
| 1K4U | L373 | P | 26.60 | 18.73 | 13.46 | 8 | 0.88 | W |
| 1K4U | I374 | P | 0.37 | 41.74 | 10.91 | 9 | 1.08 | S |
| 1K4U | R377 | P | 44.29 | 5.01 | 22.51 | 9 | 0.37 | W |
| 1K4U | T382 | P | 0.00 | 19.64 | 39.60 | 9 | 0.97 | I |
| 1LQB | M561 | D | 68.07 | 12.32 | 32.62 | 9 | 0.3 | N |
| 1LQB | L562 | D | 32.36 | 14.62 | 56.87 | 8 | 1 | N |
| 1MQ8 | T206 | B | 0.00 | 22.03 | 1.85 | 9 | 3.43 | S |
| 1NFI | Y181 | F | 4.95 | 29.11 | 63.24 | 2 | 2.35 | S |
| 1NFI | C215 | F | 14.37 | 6.35 | 61.94 | 2 | -0.08 | N |
| 1UB4 | F453 | C | 24.87 | 24.53 | 38.36 | 3 | 1.89 | N |
| 1UB4 | L455 | C | 54.02 | 19.22 | 25.62 | 8 | 1.98 | S |
| 1UB4 | L458 | C | 5.55 | 30.60 | 47.10 | 8 | 1.98 | S |
| 2HHB | Y35 | D | 21.77 | 20.20 | 5.78 | 9 | 0.18 | N |
| 2NMB | M99 | A | 26.69 | 14.40 | 10.91 | 6 | 0.24 | S |
| 2NMB | C150 | A | 6.39 | 40.73 | 13.51 | 5 | -0.01 | S |
| 2NMB | Y2 | B | 36.29 | 9.69 | 40.25 | 1 | 1.9 | I |
| 2NMB | I3 | B | 8.29 | 20.67 | 53.02 | 1 | 1.19 | I |
| 3SAK | E8 | A | 67.60 | 0.00 | 14.40 | 9 | -0.05 | W |
| 3SAK | F10 | A | 28.16 | 14.72 | 56.35 | 5 | 1.99 | S |
| 3SAK | T11 | A | 73.03 | 2.12 | 26.83 | 8 | 0.51 | I |
| 3SAK | L12 | A | 11.69 | 17.26 | 65.50 | 8 | 1.98 | S |
| 3SAK | Q13 | A | 58.13 | 4.75 | 40.10 | 5 | 0.79 | W |
| 3SAK | I14 | A | 0.00 | 28.28 | 25.65 | 9 | 0.93 | S |
| 3SAK | R15 | A | 39.13 | 14.87 | 46.03 | 8 | 0.79 | I |
| 3SAK | R17 | A | 63.61 | 8.56 | 18.86 | 5 | 0.27 | W |
| 3SAK | R19 | A | 14.24 | 20.16 | 36.16 | 7 | 1.18 | S |
| 3SAK | F20 | A | 18.93 | 23.72 | 30.21 | 1 | 1.88 | S |
| 3SAK | F23 | A | 0.75 | 34.26 | 38.21 | 4 | 2.19 | S |
| 3SAK | L26 | A | 41.26 | 20.05 | 12.63 | 4 | 0.22 | S |
| 3SAK | N27 | A | 4.99 | 16.35 | 49.35 | 9 | 0.28 | I |
| 3SAK | L30 | A | 28.46 | 22.06 | 34.57 | 9 | 0.62 | S |
| 3SAK | D34 | A | 33.23 | 12.00 | 30.13 | 7 | 0.73 | W |

&This table is derived from Tuncbag *et.al ,Bioinformatics* (2009).

1Interaction strength; W (weak), I (intermediate), N (insignificant), S (strong).

\*\* represents hotspot

-- represents non-hotspot

**6. Table S3& Training dataset derived from SKEMPI**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **PDB\_ID** | **Residue** | **Chain** | **ΔΔGcom** | **Observed** | **PDB\_ID** | **Residue** | **Chain** | **ΔΔGcom** | **Observed** |
| 1A22 | 3T | A | 0.050 | -- | 1EMV | 84S | B | 0.109 | -- |
| 1A22 | 7S | A | 0.340 | -- | 1EMV | 86F | B | 6.044 | \*\* |
| 1A22 | 8R | A | 0.200 | -- | 1EMV | 87T | B | 0.158 | -- |
| 1A22 | 9L | A | 0.040 | -- | 1EMV | 92Q | B | 0.278 | -- |
| 1A22 | 12N | A | 0.100 | -- | 1F47 | 8I | A | 2.515 | \*\* |
| 1A22 | 14M | A | 0.000 | -- | 1F47 | 9P | A | 0.058 | -- |
| 1A22 | 15L | A | 0.150 | -- | 1F47 | 11F | A | 2.444 | \*\* |
| 1A22 | 16R | A | 0.238 | -- | 1F47 | 12L | A | 2.294 | \*\* |
| 1A22 | 19R | A | 0.051 | -- | 1F47 | 14K | A | 0.043 | -- |
| 1A22 | 21H | A | 0.155 | -- | 1F47 | 15Q | A | 0.046 | -- |
| 1A22 | 22Q | A | 0.220 | -- | 1FC2 | 26F | C | 0.014 | -- |
| 1A22 | 25F | A | 0.229 | -- | 1FC2 | 27I | C | 3.729 | \*\* |
| 1A22 | 26D | A | 0.211 | -- | 1FCC | 25T | C | 0.240 | -- |
| 1A22 | 42Y | A | 0.221 | -- | 1FCC | 31K | C | 3.476 | \*\* |
| 1A22 | 46Q | A | 0.191 | -- | 1FCC | 35N | C | 2.364 | \*\* |
| 1A22 | 51S | A | 0.348 | -- | 1FCC | 40D | C | 0.272 | -- |
| 1A22 | 55S | A | 0.110 | -- | 1FCC | 42E | C | 0.385 | -- |
| 1A22 | 57S | A | 0.200 | -- | 1FCC | 43W | C | 3.771 | \*\* |
| 1A22 | 59P | A | 0.380 | -- | 1FFW | 23H | B | 0.034 | -- |
| 1A22 | 62S | A | 0.155 | -- | 1FFW | 44D | B | 0.074 | -- |
| 1A22 | 63N | A | 0.314 | -- | 1FFW | 49D | B | 0.096 | -- |
| 1A22 | 69Q | A | 0.050 | -- | 1FFW | 55C | B | 0.204 | -- |
| 1A22 | 73L | A | 0.200 | -- | 1FFW | 56F | B | 3.644 | \*\* |
| 1A22 | 153Y | A | 0.348 | -- | 1GC1 | 1K | C | 0.062 | -- |
| 1A22 | 156R | A | 0.278 | -- | 1GC1 | 2K | C | 0.017 | -- |
| 1A22 | 157K | A | 0.155 | -- | 1GC1 | 8K | C | 0.105 | -- |
| 1A22 | 161K | A | 2.014 | \*\* | 1GC1 | 10D | C | 0.000 | -- |
| 1A22 | 167R | A | 2.424 | \*\* | 1GC1 | 11T | C | 0.000 | -- |
| 1A22 | 169V | A | 0.000 | -- | 1GC1 | 15T | C | 0.322 | -- |
| 1A22 | 170Q | A | 0.270 | -- | 1GC1 | 17T | C | 0.128 | -- |
| 1A22 | 173S | A | 0.050 | -- | 1GC1 | 19S | C | 0.000 | -- |
| 1A22 | 175E | A | 0.012 | -- | 1GC1 | 20Q | C | 0.017 | -- |
| 1A22 | 176G | A | 0.340 | -- | 1GC1 | 21K | C | 0.128 | -- |
| 1A22 | 177S | A | 0.200 | -- | 1GC1 | 22K | C | 0.240 | -- |
| 1A22 | 180F | A | 0.191 | -- | 1GC1 | 23S | C | 0.293 | -- |
| 1A22 | 2K | B | 0.240 | -- | 1GC1 | 25Q | C | 0.032 | -- |
| 1A22 | 5K | B | 0.240 | -- | 1GC1 | 27H | C | 0.282 | -- |
| 1A22 | 7R | B | 0.269 | -- | 1GC1 | 30N | C | 0.170 | -- |
| 1A22 | 9P | B | 0.260 | -- | 1GC1 | 31S | C | 0.105 | -- |
| 1A22 | 15S | B | 0.015 | -- | 1GC1 | 32N | C | 0.183 | -- |
| 1A22 | 19T | B | 0.070 | -- | 1GC1 | 33Q | C | 0.105 | -- |
| 1A22 | 31N | B | 0.011 | -- | 1GC1 | 35K | C | 0.322 | -- |
| 1A22 | 32T | B | 0.077 | -- | 1GC1 | 42S | C | 0.000 | -- |
| 1A22 | 33Q | B | 0.194 | -- | 1GC1 | 45T | C | 0.149 | -- |
| 1A22 | 34E | B | 0.172 | -- | 1GC1 | 50K | C | 0.047 | -- |
| 1A22 | 36T | B | 0.025 | -- | 1GC1 | 53D | C | 0.302 | -- |
| 1A22 | 38E | B | 0.079 | -- | 1GC1 | 56D | C | 0.070 | -- |
| 1A22 | 39W | B | 0.050 | -- | 1GC1 | 58R | C | 0.132 | -- |
| 1A22 | 40K | B | 0.144 | -- | 1GC1 | 60S | C | 0.089 | -- |
| 1A22 | 50E | B | 0.178 | -- | 1GC1 | 66N | C | 0.034 | -- |
| 1A22 | 54Y | B | 0.199 | -- | 1GC1 | 72K | C | 0.017 | -- |
| 1A22 | 56N | B | 0.255 | -- | 1GC1 | 73N | C | 0.108 | -- |
| 1A22 | 57S | B | 0.161 | -- | 1GC1 | 75K | C | 0.158 | -- |
| 1A22 | 59F | B | 0.015 | -- | 1GC1 | 86V | C | 0.070 | -- |
| 1A22 | 61S | B | 0.028 | -- | 1GC1 | 87E | C | 0.218 | -- |
| 1A22 | 65P | B | 2.965 | \*\* | 1GC1 | 88D | C | 0.070 | -- |
| 1A22 | 67C | B | 0.000 | -- | 1GC1 | 89Q | C | 0.170 | -- |
| 1A22 | 69K | B | 0.043 | -- | 1GC1 | 90K | C | 0.047 | -- |
| 1A22 | 78D | B | 0.210 | -- | 1GC1 | 91E | C | 0.128 | -- |
| 1A22 | 79E | B | 0.057 | -- | 1GC1 | 92E | C | 0.016 | -- |
| 1A22 | 80K | B | 0.130 | -- | 1GC1 | 94Q | C | 0.108 | -- |
| 1A22 | 81C | B | 0.000 | -- | 1GCQ | 18P | C | 0.121 | -- |
| 1A22 | 83S | B | 0.237 | -- | 1GCQ | 19P | C | 0.085 | -- |
| 1A22 | 88V | B | 0.046 | -- | 1H9D | 94N | B | 2.110 | \*\* |
| 1A22 | 89Q | B | 0.030 | -- | 1IAR | 6T | A | 0.104 | -- |
| 1A22 | 107D | B | 0.314 | -- | 1IAR | 8Q | A | 0.022 | -- |
| 1A22 | 111R | B | 0.314 | -- | 1IAR | 11I | A | 0.069 | -- |
| 1A22 | 113E | B | 0.314 | -- | 1IAR | 15N | A | 0.034 | -- |
| 1A22 | 116R | B | 0.062 | -- | 1IAR | 16S | A | 0.183 | -- |
| 1A22 | 120I | B | 2.164 | \*\* | 1IAR | 19E | A | 0.320 | -- |
| 1A22 | 121Q | B | 0.009 | -- | 1IAR | 77K | A | 0.154 | -- |
| 1A22 | 122K | B | 0.027 | -- | 1IAR | 78Q | A | 0.125 | -- |
| 1A22 | 128E | B | 0.083 | -- | 1IAR | 82F | A | 0.086 | -- |
| 1A22 | 130E | B | 0.079 | -- | 1IAR | 84K | A | 0.345 | -- |
| 1A22 | 134K | B | 0.000 | -- | 1IAR | 88R | A | 3.753 | \*\* |
| 1A22 | 135E | B | 0.199 | -- | 1JCK | 90Y | B | 2.595 | \*\* |
| 1A22 | 138E | B | 0.120 | -- | 1JCK | 91V | B | 2.232 | \*\* |
| 1A22 | 140K | B | 0.120 | -- | 1JCK | 176F | B | 2.133 | \*\* |
| 1A22 | 142K | B | 0.120 | -- | 1JRH | 37K | I | 3.714 | \*\* |
| 1A22 | 145D | B | 0.120 | -- | 1JRH | 38N | I | 0.170 | -- |
| 1A22 | 149T | B | 0.202 | -- | 1JRH | 39Y | I | 3.527 | \*\* |
| 1A22 | 150T | B | 0.097 | -- | 1JRH | 40G | I | 4.450 | \*\* |
| 1A22 | 166R | B | 0.056 | -- | 1JRH | 42K | I | 3.386 | \*\* |
| 1A22 | 168R | B | 0.190 | -- | 1JRH | 43N | I | 4.299 | \*\* |
| 1A22 | 172R | B | 0.268 | -- | 1JRH | 44S | I | 0.378 | -- |
| 1A22 | 173N | B | 0.298 | -- | 1JRH | 69N | I | 0.200 | -- |
| 1A22 | 174S | B | 0.034 | -- | 1JRH | 71L | I | 2.959 | \*\* |
| 1A22 | 179E | B | 0.108 | -- | 1JRH | 72W | I | 4.429 | \*\* |
| 1A4Y | 5R | B | 6.936 | \*\* | 1JRH | 73V | I | 0.214 | -- |
| 1A4Y | 12Q | B | 0.300 | -- | 1JRH | 74R | I | 0.393 | -- |
| 1A4Y | 13H | B | 0.297 | -- | 1JRH | 88K | I | 0.312 | -- |
| 1A4Y | 31R | B | 0.250 | -- | 1JRH | 92W | L | 2.818 | \*\* |
| 1A4Y | 33R | B | 0.327 | -- | 1JRH | 94T | L | 0.385 | -- |
| 1A4Y | 66R | B | 0.203 | -- | 1JRH | 54W | H | 2.686 | \*\* |
| 1A4Y | 68N | B | 0.118 | -- | 1JRH | 55W | H | 2.421 | \*\* |
| 1A4Y | 70R | B | 0.232 | -- | 1JRH | 103F | H | 0.000 | -- |
| 1A4Y | 84H | B | 0.170 | -- | 1JTG | 36F | B | 3.415 | \*\* |
| 1A4Y | 89W | B | 0.240 | -- | 1JTG | 41H | B | 2.950 | \*\* |
| 1A4Y | 108E | B | 0.323 | -- | 1JTG | 53Y | B | 2.690 | \*\* |
| 1A4Y | 261W | A | 0.101 | -- | 1JTG | 71S | B | 2.520 | \*\* |
| 1A4Y | 287E | A | 0.101 | -- | 1JTG | 74K | B | 3.906 | \*\* |
| 1A4Y | 289S | A | 0.042 | -- | 1JTG | 112W | B | 3.033 | \*\* |
| 1A4Y | 320K | A | 0.310 | -- | 1JTG | 113S | B | 2.286 | \*\* |
| 1A4Y | 344E | A | 0.179 | -- | 1JTG | 142F | B | 3.546 | \*\* |
| 1A4Y | 430Q | A | 0.072 | -- | 1JTG | 143Y | B | 3.138 | \*\* |
| 1A4Y | 432V | A | 0.072 | -- | 1JTG | 148H | B | 2.683 | \*\* |
| 1A4Y | 434Y | A | 7.207 | \*\* | 1JTG | 150W | B | 4.132 | \*\* |
| 1A4Y | 435D | A | 6.248 | \*\* | 1JTG | 160R | B | 2.631 | \*\* |
| 1A4Y | 437Y | A | 6.315 | \*\* | 1JTG | 162W | B | 2.727 | \*\* |
| 1A4Y | 457R | A | 0.224 | -- | 1JTG | 74Q | A | 2.972 | \*\* |
| 1AHW | 156T | C | 0.074 | -- | 1JTG | 75N | A | 2.142 | \*\* |
| 1AHW | 187V | C | 0.314 | -- | 1JTG | 78V | A | 3.750 | \*\* |
| 1AK4 | 85P | D | 2.449 | \*\* | 1JTG | 79E | A | 2.080 | \*\* |
| 1AK4 | 86V | D | 2.355 | \*\* | 1JTG | 80Y | A | 2.276 | \*\* |
| 1AK4 | 87H | D | 2.373 | \*\* | 1JTG | 85E | A | 4.529 | \*\* |
| 1AK4 | 89G | D | 3.440 | \*\* | 1JTG | 104M | A | 2.001 | \*\* |
| 1AK4 | 90P | D | 3.535 | \*\* | 1JTG | 105S | A | 2.039 | \*\* |
| 1AK4 | 93P | D | 2.046 | \*\* | 1JTG | 143E | A | 2.421 | \*\* |
| 1BRS | 25K | A | 6.484 | \*\* | 1JTG | 190V | A | 0.302 | -- |
| 1BRS | 56N | A | 3.089 | \*\* | 1JTG | 208K | A | 2.648 | \*\* |
| 1BRS | 57R | A | 6.526 | \*\* | 1JTG | 217R | A | 2.459 | \*\* |
| 1BRS | 58E | A | 0.094 | -- | 1KTZ | 64R | A | 2.883 | \*\* |
| 1BRS | 71E | A | 4.135 | \*\* | 1KTZ | 3L | B | 2.270 | \*\* |
| 1BRS | 85R | A | 6.723 | \*\* | 1KTZ | 6F | B | 3.425 | \*\* |
| 1BRS | 100H | A | 6.935 | \*\* | 1KTZ | 26I | B | 2.342 | \*\* |
| 1BRS | 29Y | D | 7.141 | \*\* | 1LFD | 35K | A | 0.258 | -- |
| 1BRS | 35D | D | 6.575 | \*\* | 1LFD | 43D | A | 0.280 | -- |
| 1BRS | 39D | D | 7.666 | \*\* | 1LFD | 44E | A | 0.246 | -- |
| 1BRS | 42T | D | 5.941 | \*\* | 1MAH | 327Y | A | 0.386 | -- |
| 1BRS | 74E | D | 4.673 | \*\* | 1NMB | 103Y | H | 2.140 | \*\* |
| 1BRS | 78E | D | 4.327 | \*\* | 1PPF | 14P | I | 0.122 | -- |
| 1CBW | 11T | I | 0.220 | -- | 1PPF | 17T | I | 3.145 | \*\* |
| 1CBW | 13P | I | 0.056 | -- | 1PPF | 18L | I | 3.541 | \*\* |
| 1CBW | 15K | I | 2.091 | \*\* | 1PPF | 20Y | I | 3.166 | \*\* |
| 1CBW | 19I | I | 0.141 | -- | 1PPF | 21R | I | 0.205 | -- |
| 1CBW | 20R | I | 0.350 | -- | 1PPF | 42V | I | 2.581 | \*\* |
| 1CBW | 33F | I | 0.141 | -- | 1R0R | 13L | I | 3.775 | \*\* |
| 1CBW | 34V | I | 0.051 | -- | 1R0R | 14E | I | 2.060 | \*\* |
| 1CBW | 39R | I | 0.220 | -- | 1R0R | 15Y | I | 5.398 | \*\* |
| 1CBW | 46K | I | 0.141 | -- | 1R0R | 16R | I | 0.095 | -- |
| 1CHO | 10K | I | 0.179 | -- | 1R0R | 27G | I | 3.081 | \*\* |
| 1CHO | 11P | I | 0.375 | -- | 1R0R | 31N | I | 0.033 | -- |
| 1CHO | 14T | I | 4.179 | \*\* | 1REW | 38F | A | 2.123 | \*\* |
| 1CHO | 15L | I | 6.271 | \*\* | 1REW | 39P | A | 2.088 | \*\* |
| 1CHO | 16E | I | 2.301 | \*\* | 1REW | 42D | A | 0.065 | -- |
| 1CHO | 17Y | I | 2.508 | \*\* | 1REW | 77S | A | 0.193 | -- |
| 1CHO | 18R | I | 3.147 | \*\* | 1REW | 89L | A | 0.176 | -- |
| 1CHO | 39V | I | 5.095 | \*\* | 1REW | 38F | B | 2.123 | \*\* |
| 1DAN | 10K | T | 0.397 | -- | 1REW | 39P | B | 2.088 | \*\* |
| 1DAN | 11S | T | 0.130 | -- | 1REW | 42D | B | 0.065 | -- |
| 1DAN | 12T | T | 0.120 | -- | 1REW | 77S | B | 0.193 | -- |
| 1DAN | 13N | T | 0.180 | -- | 1REW | 89L | B | 0.176 | -- |
| 1DAN | 15K | T | 3.664 | \*\* | 1REW | 55Q | C | 2.657 | \*\* |
| 1DAN | 16T | T | 0.159 | -- | 1S1Q | 42F | A | 0.196 | -- |
| 1DAN | 21E | T | 0.101 | -- | 1S1Q | 73W | A | 0.276 | -- |
| 1DAN | 23K | T | 0.117 | -- | 1TM1 | 39T | I | 2.896 | \*\* |
| 1DAN | 28V | T | 0.193 | -- | 1TM1 | 41E | I | 2.530 | \*\* |
| 1DAN | 31V | T | 0.132 | -- | 1TM1 | 42Y | I | 2.579 | \*\* |
| 1DAN | 33I | T | 0.132 | -- | 1TM1 | 46R | I | 3.960 | \*\* |
| 1DAN | 37S | T | 0.069 | -- | 1TM1 | 48R | I | 3.689 | \*\* |
| 1DAN | 38G | T | 0.067 | -- | 1TM1 | 51V | I | 0.025 | -- |
| 1DAN | 39D | T | 2.945 | \*\* | 1VFB | 92W | A | 3.357 | \*\* |
| 1DAN | 42S | T | 0.044 | -- | 1VFB | 93S | A | 0.343 | -- |
| 1DAN | 46Y | T | 0.132 | -- | 1VFB | 30T | B | 0.056 | -- |
| 1DAN | 53D | T | 3.000 | \*\* | 1VFB | 56N | B | 0.178 | -- |
| 1DAN | 54L | T | 0.000 | -- | 1VFB | 58D | B | 0.207 | -- |
| 1DAN | 55T | T | 3.577 | \*\* | 1VFB | 99R | B | 0.100 | -- |
| 1DAN | 56D | T | 0.273 | -- | 1VFB | 100D | B | 3.126 | \*\* |
| 1DAN | 57E | T | 0.152 | -- | 1VFB | 19N | C | 0.396 | -- |
| 1DAN | 58I | T | 0.000 | -- | 1VFB | 24S | C | 2.110 | \*\* |
| 1DAN | 59V | T | 0.000 | -- | 1VFB | 121Q | C | 2.660 | \*\* |
| 1DAN | 63K | T | 0.138 | -- | 1VFB | 124I | C | 2.662 | \*\* |
| 1DAN | 64Q | T | 0.103 | -- | 1VFB | 125R | C | 2.615 | \*\* |
| 1DAN | 67L | T | 0.060 | -- | 1XD3 | 8L | B | 2.738 | \*\* |
| 1DAN | 2P | U | 0.193 | -- | 1XD3 | 24E | B | 0.246 | -- |
| 1DAN | 9E | U | 0.175 | -- | 1XD3 | 27K | B | 0.064 | -- |
| 1DAN | 15E | U | 0.261 | -- | 1XD3 | 44I | B | 0.272 | -- |
| 1DAN | 16T | U | 0.060 | -- | 1XD3 | 52D | B | 0.246 | -- |
| 1DAN | 17N | U | 0.207 | -- | 1XD3 | 58D | B | 0.246 | -- |
| 1DAN | 24Q | U | 0.034 | -- | 1Z7X | 263W | W | 2.211 | \*\* |
| 1DAN | 27E | U | 0.034 | -- | 1Z7X | 434Y | W | 6.786 | \*\* |
| 1DAN | 32K | U | 0.121 | -- | 1Z7X | 435D | W | 5.414 | \*\* |
| 1DAN | 38E | U | 0.086 | -- | 1Z7X | 437Y | W | 4.930 | \*\* |
| 1DAN | 39D | U | 0.027 | -- | 1Z7X | 459I | W | 0.337 | -- |
| 1DAN | 40E | U | 0.022 | -- | 2FTL | 12G | I | 4.346 | \*\* |
| 1DAN | 41R | U | 0.000 | -- | 2FTL | 15K | I | 10.289 | \*\* |
| 1DAN | 42T | U | 0.000 | -- | 2FTL | 18I | I | 4.969 | \*\* |
| 1DAN | 43L | U | 0.028 | -- | 2FTL | 36G | I | 2.191 | \*\* |
| 1DAN | 46R | U | 0.073 | -- | 2G2U | 36F | B | 2.762 | \*\* |
| 1DAN | 47N | U | 0.206 | -- | 2G2U | 50Y | B | 2.200 | \*\* |
| 1DAN | 48N | U | 0.103 | -- | 2G2U | 53Y | B | 2.301 | \*\* |
| 1DAN | 49T | U | 0.017 | -- | 2G2U | 73E | B | 2.088 | \*\* |
| 1DAN | 50F | U | 3.451 | \*\* | 2G2U | 74K | B | 0.217 | -- |
| 1DAN | 54R | U | 0.003 | -- | 2G2U | 112W | B | 0.274 | -- |
| 1DAN | 55D | U | 0.011 | -- | 2G2U | 142F | B | 0.276 | -- |
| 1DAN | 56V | U | 0.199 | -- | 2G2U | 144R | B | 0.342 | -- |
| 1DAN | 57F | U | 0.060 | -- | 2I9B | 129R | E | 0.287 | -- |
| 1DAN | 59K | U | 0.101 | -- | 2I9B | 134R | E | 0.363 | -- |
| 1DAN | 60D | U | 0.101 | -- | 2J0T | 2T | D | 4.387 | \*\* |
| 1DAN | 62I | U | 0.179 | -- | 2J0T | 68S | D | 3.694 | \*\* |
| 1DAN | 67Y | U | 0.000 | -- | 2J1K | 155R | C | 0.052 | -- |
| 1DAN | 69S | U | 0.023 | -- | 2JEL | 62T | P | 0.000 | -- |
| 1DAN | 71K | U | 0.240 | -- | 2JEL | 70E | P | 2.727 | \*\* |
| 1DAN | 72K | U | 0.240 | -- | 2JEL | 83E | P | 0.000 | -- |
| 1DAN | 73T | U | 0.212 | -- | 2JEL | 85E | P | 0.000 | -- |
| 1DAN | 75K | U | 0.117 | -- | 2O3B | 24E | B | 5.472 | \*\* |
| 1DAN | 78T | U | 0.026 | -- | 2O3B | 74Q | B | 4.492 | \*\* |
| 1DAN | 79N | U | 0.025 | -- | 2O3B | 76W | B | 4.912 | \*\* |
| 1DAN | 80E | U | 0.025 | -- | 2PCC | 34D | A | 0.264 | -- |
| 1DAN | 82L | U | 0.080 | -- | 2PCC | 197V | A | 2.126 | \*\* |
| 1DAN | 85V | U | 0.110 | -- | 2PCC | 290E | A | 3.650 | \*\* |
| 1DAN | 87K | U | 0.017 | -- | 2QJA | 43T | C | 0.097 | -- |
| 1DAN | 89E | U | 0.094 | -- | 2QJA | 62P | C | 0.268 | -- |
| 1DAN | 90N | U | 0.094 | -- | 2SIC | 67M | I | 0.218 | -- |
| 1DAN | 91Y | U | 0.330 | -- | 2VLJ | 52D | E | 0.132 | -- |
| 1DAN | 101S | U | 0.318 | -- | 2VLJ | 95S | E | 0.035 | -- |
| 1DAN | 103T | U | 0.020 | -- | 2VLJ | 97Y | E | 0.232 | -- |
| 1DAN | 104V | U | 0.020 | -- | 2WPT | 30D | A | 0.132 | -- |
| 1DAN | 105N | U | 0.200 | -- | 2WPT | 34V | A | 3.459 | \*\* |
| 1DAN | 106R | U | 0.400 | -- | 2WPT | 38E | A | 4.501 | \*\* |
| 1DAN | 107K | U | 0.043 | -- | 2WPT | 39R | A | 0.240 | -- |
| 1DAN | 109T | U | 0.135 | -- | 2WPT | 47S | A | 2.424 | \*\* |
| 1DAN | 110D | U | 0.043 | -- | 2WPT | 53P | A | 2.926 | \*\* |
| 1DAN | 114E | U | 0.005 | -- | 2WPT | 67S | B | 0.134 | -- |
| 1DAN | 135L | H | 0.016 | -- | 2WPT | 71S | B | 0.095 | -- |
| 1DAN | 189K | H | 0.185 | -- | 2WPT | 77S | B | 0.067 | -- |
| 1DQJ | 20Y | C | 3.814 | \*\* | 2WPT | 80T | B | 0.376 | -- |
| 1DQJ | 21R | C | 2.271 | \*\* | 2WPT | 85Q | B | 0.384 | -- |
| 1DQJ | 96K | C | 5.978 | \*\* | 2WPT | 91V | B | 0.265 | -- |
| 1DQJ | 97K | C | 3.705 | \*\* | 3BK3 | 2L | C | 0.000 | -- |
| 1DQJ | 100S | C | 2.350 | \*\* | 3BN9 | 26I | B | 0.000 | -- |
| 1DQJ | 31N | A | 2.013 | \*\* | 3BN9 | 47D | B | 0.311 | -- |
| 1DQJ | 32N | A | 4.946 | \*\* | 3BN9 | 48R | B | 0.045 | -- |
| 1DQJ | 50Y | A | 2.678 | \*\* | 3BN9 | 50F | B | 0.045 | -- |
| 1DQJ | 91S | A | 2.725 | \*\* | 3BN9 | 51R | B | 0.072 | -- |
| 1DQJ | 33Y | B | 5.524 | \*\* | 3BN9 | 52Y | B | 0.019 | -- |
| 1DQJ | 50Y | B | 6.887 | \*\* | 3BN9 | 82R | B | 0.159 | -- |
| 1DQJ | 98W | B | 5.516 | \*\* | 3BN9 | 138H | B | 0.085 | -- |
| 1DVF | 32Y | A | 2.904 | \*\* | 3BN9 | 140Q | B | 0.133 | -- |
| 1DVF | 49Y | A | 2.003 | \*\* | 3BN9 | 144T | B | 0.291 | -- |
| 1DVF | 92W | A | 0.341 | -- | 3BN9 | 147L | B | 0.336 | -- |
| 1DVF | 52W | B | 4.143 | \*\* | 3BN9 | 163E | B | 0.373 | -- |
| 1DVF | 54D | B | 4.351 | \*\* | 3BN9 | 168Q | B | 0.035 | -- |
| 1DVF | 98E | B | 4.335 | \*\* | 3BN9 | 169Q | B | 2.509 | \*\* |
| 1DVF | 100D | B | 3.627 | \*\* | 3BN9 | 219R | B | 0.094 | -- |
| 1DVF | 33H | D | 2.790 | \*\* | 3BP8 | 115F | A | 0.033 | -- |
| 1DVF | 52D | D | 3.001 | \*\* | 3HFM | 20Y | Y | 5.400 | \*\* |
| 1DVF | 55N | D | 2.570 | \*\* | 3HFM | 21R | Y | 3.911 | \*\* |
| 1DVF | 101I | D | 2.681 | \*\* | 3HFM | 63W | Y | 0.319 | -- |
| 1DVF | 102Y | D | 4.686 | \*\* | 3HFM | 73R | Y | 0.331 | -- |
| 1DVF | 104Q | D | 2.185 | \*\* | 3HFM | 89T | Y | 0.000 | -- |
| 1DVF | 106R | D | 4.370 | \*\* | 3HFM | 93N | Y | 0.211 | -- |
| 1DVF | 49Y | C | 3.176 | \*\* | 3HFM | 96K | Y | 7.428 | \*\* |
| 1EAW | 45I | A | 0.194 | -- | 3HFM | 97K | Y | 5.705 | \*\* |
| 1EAW | 46D | A | 0.172 | -- | 3HFM | 98I | Y | 0.000 | -- |
| 1EAW | 51R | A | 0.231 | -- | 3HFM | 100S | Y | 0.268 | -- |
| 1EAW | 52Y | A | 0.079 | -- | 3HFM | 31N | L | 6.341 | \*\* |
| 1EAW | 82R | A | 0.150 | -- | 3HFM | 32N | L | 5.107 | \*\* |
| 1EAW | 90N | A | 0.308 | -- | 3HFM | 50Y | L | 6.493 | \*\* |
| 1EAW | 93T | A | 0.255 | -- | 3HFM | 96Y | L | 4.232 | \*\* |
| 1EAW | 138H | A | 0.014 | -- | 3HFM | 31S | H | 0.170 | -- |
| 1EAW | 140Q | A | 0.307 | -- | 3HFM | 32D | H | 2.538 | \*\* |
| 1EAW | 144T | A | 0.089 | -- | 3HFM | 33Y | H | 6.631 | \*\* |
| 1EAW | 169Q | A | 0.133 | -- | 3HFM | 50Y | H | 7.630 | \*\* |
| 1EAW | 214D | A | 2.228 | \*\* | 3HFM | 53Y | H | 3.250 | \*\* |
| 1EAW | 218Q | A | 0.144 | -- | 3HFM | 98W | H | 6.620 | \*\* |
| 1EAW | 219R | A | 0.089 | -- | 3NPS | 23Q | A | 0.026 | -- |
| 1EMV | 22N | A | 0.139 | -- | 3NPS | 45I | A | 0.332 | -- |
| 1EMV | 24D | A | 0.337 | -- | 3NPS | 46D | A | 0.340 | -- |
| 1EMV | 26S | A | 3.196 | \*\* | 3NPS | 50F | A | 0.220 | -- |
| 1EMV | 29E | A | 0.307 | -- | 3NPS | 51R | A | 0.138 | -- |
| 1EMV | 30E | A | 0.220 | -- | 3NPS | 82R | A | 0.152 | -- |
| 1EMV | 31L | A | 5.047 | \*\* | 3NPS | 90N | A | 0.253 | -- |
| 1EMV | 32V | A | 3.621 | \*\* | 3NPS | 140Q | A | 0.296 | -- |
| 1EMV | 33K | A | 0.192 | -- | 3NPS | 144T | A | 0.175 | -- |
| 1EMV | 35V | A | 2.865 | \*\* | 3NPS | 147L | A | 0.296 | -- |
| 1EMV | 39E | A | 2.083 | \*\* | 3NPS | 168Q | A | 0.059 | -- |
| 1EMV | 42T | A | 0.305 | -- | 3NPS | 218Q | A | 0.041 | -- |
| 1EMV | 43E | A | 0.213 | -- | 3NPS | 219R | A | 0.084 | -- |
| 1EMV | 46S | A | 0.007 | -- | 3NPS | 221K | A | 0.104 | -- |
| 1EMV | 48S | A | 2.187 | \*\* | 3SGB | 7K | I | 2.536 | \*\* |
| 1EMV | 49D | A | 5.915 | \*\* | 3SGB | 8P | I | 0.187 | -- |
| 1EMV | 52Y | A | 6.776 | \*\* | 3SGB | 11T | I | 3.363 | \*\* |
| 1EMV | 53Y | A | 6.447 | \*\* | 3SGB | 12L | I | 3.533 | \*\* |
| 1EMV | 67N | A | 0.278 | -- | 3SGB | 15R | I | 0.053 | -- |
| 1EMV | 74S | B | 0.241 | -- | 3SGB | 30N | I | 0.326 | -- |
| 1EMV | 75N | B | 2.334 | \*\* | 3SGB | 36V | I | 2.713 | \*\* |
| 1EMV | 77S | B | 0.233 | -- | 4CPA | 37V | I | 2.324 | \*\* |

\*\* represents hotspot

-- represents non-hotspot

& SKEMPI data is obtained by computing binding free energy change(∆∆G), so the value of the same residue of protein on other databases is a little different.

**7. Table S4 SKEMPIs Dataset**

This datasets removed the same sequences of protein in ASEdb database. Table S4 lists all PDB ID of used proteins.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **PDB\_ID** | **Chain** | **PDB\_ID** | **Chain** | **PDB\_ID** | **Chain** | **PDB\_ID** | **Chain** | **PDB\_ID** | **Chain** |
| 1A22 | A,B | 1FC2 | C | 1LFD | A | 2FTL | I | 2VLJ | E |
| 1AK4 | D | 1FCC& | C | 1MAH | A | 2G2U | B | 2WPT | A |
| 1CBW | I | 1FFW | B | 1PPF | I | 2I9B | E | 2WPT | B |
| 1DAN | H | 1GCQ | C | 1R0R | I | 2J0T | D | 3BK3 | C |
| 1DQJ | A,B,C | 1H9D | B | 1REW | A,B,C | 2J1K | C | 3BN9 | B |
| 1DVF | C | 1HE8 | A | 1S1Q | A | 2JEL | P | 3BP8 | A |
| 1EAW | A | 1IAR | A | 1TM1 | I | 2O3B | B | 3NPS | A |
| 1EFN | A | 1JCK | B | 1VFB | A,C | 2PCC | A | 3SGB | I |
| 1EMV | A,B | 1JRH | H,I,L | 1XD3 | B | 2QJA | C | 4CPA | I |
| 1F47 | A | 1KTZ | A,B | 1Z7X | W | 2SIC | I |  |  |

& BID dataset has the same protein, so it is removed in mixed dataset

**8. Mixed Dataset**

Similarly, we removed the same proteins. That is, SKEMPIs dataset removing 1FCC protein which incorporates ASEdb and BID database to make up a new mixed dataset to validate our model.