## Online Supporting Information S5: Accuracy in IFS (incremental feature selection)

| Index | The last added feature                          | Accuracy of positive pathway | Accuracy of negative pathway | Total<br>accuracy |
|-------|---|------------------------------|------------------------------|-------------------|
| 1     | out_local_density_0.6_mean                      | 100.00%                      | 0.00%                        | 0.99%             |
| 2     | polarity_composition_P_max                      | 42. 60%                      | 95. 88%                      | 95. 35%           |
| 3     | in_local_density_0.7_max                        | 54. 44%                      | 98. 91%                      | 98. 47%           |
| 4     | in_local_density_0.5_mean                       | 58. 58%                      | 99. 27%                      | 98. 87%           |
| 5     | topological_change_0.6_0.7                      | 69. 23%                      | 99. 48%                      | 99. 18%           |
| 6     | topological_change_0.1_0.2                      | 76. 33%                      | 99. 57%                      | 99. 34%           |
| 7     | in_degree_variance                              | 73. 37%                      | 99. 59%                      | 99. 33%           |
| 8     | topological_change_0.7_0.8                      | 75. 74%                      | 99. 62%                      | 99. 38%           |
| 9     | out_local_density_0.8_mean                      | 73. 96%                      | 99. 62%                      | 99. 37%           |
| 10    | secondary_structure_distrib<br>ution_P-1.0_mean | 75. 74%                      | 99. 66%                      | 99. 43%           |

| 11 | topological_change_0.2_0.3                     | 75. 15% | 99. 68% | 99. 44% |
|----|--|---------|---------|---------|
| 12 | in_local_density_0.6_mean                      | 74. 56% | 99. 65% | 99. 40% |
| 13 | out_degree_variance                            | 75. 15% | 99. 63% | 99. 39% |
| 14 | secondary_structure_distrib<br>ution_P-1.0_max | 74. 56% | 99. 66% | 99. 41% |
| 15 | out_local_density_0.5_mean                     | 75. 74% | 99. 65% | 99. 41% |
| 16 | out_degree_correlation_max                     | 77. 51% | 99. 66% | 99. 44% |
| 17 | out_local_density_0.7_max                      | 78. 11% | 99. 65% | 99. 44% |
| 18 | polarizability_distribution<br>_N-1.0_max      | 76. 92% | 99. 66% | 99. 44% |
| 19 | in_local_density_0.7_mean                      | 78. 11% | 99. 67% | 99. 46% |
| 20 | AA_composition_C_mean                          | 79. 88% | 99. 69% | 99. 49% |
| 21 | in_degree_correlation_varia<br>nce             | 79. 88% | 99. 69% | 99. 49% |

| 22 | secondary_structure_distrib<br>ution_P-0.0_max | 79. 88% | 99. 69% | 99. 49% |
|----|--|---------|---------|---------|
| 23 | out_local_density_0.7_mean                     | 77. 51% | 99. 66% | 99. 44% |
| 24 | AA_composition_S_mean                          | 77. 51% | 99. 70% | 99. 48% |
| 25 | out_degree_correlation_vari<br>ance            | 77. 51% | 99. 70% | 99. 48% |
| 26 | VanDerWaal_distribution_P-1 .0_max             | 77. 51% | 99. 70% | 99. 48% |
| 27 | polarity_distribution_P-1.0<br>_max            | 77. 51% | 99. 71% | 99. 49% |
| 28 | in_local_density_0.8_mean                      | 74. 56% | 99. 67% | 99. 42% |
| 29 | AA_composition_K_mean                          | 73. 96% | 99. 66% | 99. 41% |
| 30 | polarity_distribution_H-1.0<br>_max            | 73. 96% | 99. 67% | 99. 42% |
| 31 | polarizability_transition_P<br>H_mean          | 74. 56% | 99. 68% | 99. 43% |
| 32 | in_clustering_max                              | 76. 33% | 99. 63% | 99. 40% |

| 33 | hydrophobicity_distribution<br>_N-1.0_max         | 76. 33% | 99. 66% | 99. 43% |
|----|---|---------|---------|---------|
| 34 | solvent_accessibility_compo<br>sition_H_max       | 76. 33% | 99. 68% | 99. 45% |
| 35 | out_local_density_0.9_mean                        | 76. 92% | 99. 63% | 99. 40% |
| 36 | VanDerWaal_distribution_N-1 .0_max                | 76. 92% | 99. 65% | 99. 42% |
| 37 | secondary_structure_transit<br>ion_PH_mean        | 74. 56% | 99. 67% | 99. 42% |
| 38 | in_local_density_0.3_mean                         | 77. 51% | 99. 67% | 99. 46% |
| 39 | hydrophobicity_distribution<br>_H-1.0_max         | 76. 92% | 99. 69% | 99. 46% |
| 40 | in_local_density_0.9_mean                         | 77. 51% | 99. 66% | 99. 44% |
| 41 | out_local_density_0_max                           | 77. 51% | 99. 64% | 99. 42% |
| 42 | solvent_accessibility_distr<br>ibution_H-1.0_mean | 76. 92% | 99. 61% | 99. 38% |

| 43 | in_local_density_0.6_max                          | 76. 33% | 99. 64% | 99. 41% |
|----|---|---------|---------|---------|
| 44 | AA_composition_V_mean                             | 76. 33% | 99. 61% | 99. 38% |
| 45 | VanDerWaal_distribution_H-1 .0_max                | 76. 33% | 99. 63% | 99. 40% |
| 46 | polarizability_distribution<br>_P-1.0_max         | 75. 74% | 99. 67% | 99. 43% |
| 47 | out_local_density_0.6_max                         | 75. 15% | 99. 66% | 99. 41% |
| 48 | hydrophobicity_distribution<br>_P-1.0_max         | 75. 15% | 99. 66% | 99. 42% |
| 49 | solvent_accessibility_distr<br>ibution_H-0.5_mean | 75. 74% | 99. 66% | 99. 43% |
| 50 | secondary_structure_distrib<br>ution_H-0.0_mean   | 75. 74% | 99. 64% | 99. 40% |
| 51 | in_local_density_0_max                            | 75. 15% | 99. 64% | 99. 40% |
| 52 | solvent_accessibility_compo<br>sition_H_mean      | 74. 56% | 99. 65% | 99. 40% |

| 53 | out_degree_correlation_mean           | 75. 15% | 99. 67% | 99. 43% |
|----|---------------------------------------|---------|---------|---------|
| 54 | out_out_topological_varianc<br>e      | 75. 74% | 99. 64% | 99. 40% |
| 55 | AA_composition_W_mean                 | 73. 37% | 99. 60% | 99. 34% |
| 56 | out_local_density_0.8_max             | 71.60%  | 99. 60% | 99. 33% |
| 57 | out_local_density_0.1_max             | 71.60%  | 99. 60% | 99. 33% |
| 58 | hydrophobicity_transition_P<br>H_mean | 71. 60% | 99. 63% | 99. 35% |
| 59 | polarity_distribution_N-1.0<br>_max   | 71. 60% | 99. 63% | 99. 35% |
| 60 | in_local_density_0.8_max              | 71.60%  | 99. 62% | 99. 34% |
| 61 | VanDerWaal_transition_PN_me<br>an     | 72. 19% | 99. 60% | 99. 33% |
| 62 | out_clustering_max                    | 72. 78% | 99. 62% | 99. 36% |
| 63 | AA_composition_L_mean                 | 72. 78% | 99. 61% | 99. 34% |
| 64 | in_local_density_0.1_max              | 72. 78% | 99. 60% | 99. 33% |

| 65 | secondary_structure_distrib<br>ution_P-0.0_mean  | 72. 78% | 99. 60% | 99. 33% |
|----|--|---------|---------|---------|
| 66 | out_local_density_0.3_mean                       | 71.60%  | 99. 60% | 99. 32% |
| 67 | AA_composition_A_mean                            | 71. 01% | 99. 62% | 99. 33% |
| 68 | AA_composition_H_mean                            | 71.60%  | 99. 57% | 99. 29% |
| 69 | polarizability_distribution<br>_H-1.0_max        | 71.60%  | 99. 57% | 99. 29% |
| 70 | VanDerWaal_distribution_H-0<br>.5_mean           | 72. 19% | 99. 57% | 99. 30% |
| 71 | in_in_topological_variance                       | 71. 01% | 99. 57% | 99. 29% |
| 72 | AA_composition_G_mean                            | 71. 60% | 99. 56% | 99. 28% |
| 73 | secondary_structure_distrib<br>ution_P-0.75_mean | 71. 01% | 99. 54% | 99. 26% |
| 74 | in_degree_correlation_mean                       | 71. 01% | 99. 55% | 99. 27% |

| 75 | secondary_structure_distrib<br>ution_N-1.0_max   | 71. 01% | 99. 54% | 99. 26% |
|----|--|---------|---------|---------|
| 76 | AA_composition_T_mean                            | 72. 19% | 99. 52% | 99. 25% |
| 77 | polarity_distribution_H-1.0<br>_mean             | 71. 01% | 99. 50% | 99. 22% |
| 78 | out_local_density_0.9_max                        | 70. 41% | 99. 51% | 99. 22% |
| 79 | secondary_structure_distrib<br>ution_N-0.5_mean  | 70. 41% | 99. 49% | 99. 20% |
| 80 | in_local_density_0.9_max                         | 70. 41% | 99. 48% | 99. 19% |
| 81 | in_local_density_0.4_mean                        | 72. 19% | 99. 50% | 99. 23% |
| 82 | secondary_structure_distrib<br>ution_H-1.0_mean  | 72. 19% | 99. 48% | 99. 21% |
| 83 | polarizability_distribution<br>_N-0.75_mean      | 71. 60% | 99. 47% | 99. 19% |
| 84 | solvent_accessibility_distr<br>ibution_H-0.0_max | 70. 41% | 99. 49% | 99. 20% |

| 85 | solvent_accessibility_distr<br>ibution_H-0.25_mean | 72. 19% | 99. 48% | 99. 21% |
|----|--|---------|---------|---------|
| 86 | AA_composition_D_mean                              | 71.60%  | 99. 46% | 99. 18% |
| 87 | out_local_density_0.2_max                          | 71.60%  | 99. 46% | 99. 19% |
| 88 | polarizability_distribution<br>_H-1.0_mean         | 71. 01% | 99. 45% | 99. 17% |
| 89 | polarizability_distribution<br>_P-1.0_mean         | 69. 82% | 99. 44% | 99. 14% |
| 90 | in_degree_max                                      | 69. 82% | 99. 45% | 99. 16% |
| 91 | weight_edge_mean(with_missing_edge)                | 70. 41% | 99. 46% | 99. 17% |
| 92 | hydrophobicity_distribution<br>_P-0.0_mean         | 70. 41% | 99. 45% | 99. 16% |
| 93 | secondary_structure_transit<br>ion_PN_mean         | 70. 41% | 99. 44% | 99. 15% |
| 94 | out_clustering_mean                                | 69. 82% | 99. 44% | 99. 15% |

| 95  | polarizability_distribution<br>_N-0.25_mean        | 71. 01% | 99. 43% | 99. 15% |
|-----|--|---------|---------|---------|
| 96  | secondary_structure_distrib<br>ution_H-0.5_mean    | 69. 82% | 99. 43% | 99. 14% |
| 97  | AA_composition_Q_mean                              | 69. 23% | 99. 42% | 99. 12% |
| 98  | solvent_accessibility_distr<br>ibution_H-0.75_mean | 68. 64% | 99. 40% | 99. 09% |
| 99  | AA_composition_P_mean                              | 69. 23% | 99. 40% | 99. 10% |
| 100 | secondary_structure_distrib<br>ution_P-0.25_mean   | 68. 64% | 99. 41% | 99. 10% |
| 101 | hydrophobicity_composition_<br>H_max               | 70. 41% | 99. 43% | 99. 14% |
| 102 | polarity_distribution_H-0.2<br>5_mean              | 71. 01% | 99. 41% | 99. 13% |
| 103 | AA_composition_N_mean                              | 71. 01% | 99. 41% | 99. 13% |

| 104 | hydrophobicity_distribution<br>_N-0.0_mean  | 69. 82% | 99. 39% | 99. 10% |
|-----|---|---------|---------|---------|
| 105 | in_local_density_0.2_max                    | 69. 82% | 99. 38% | 99. 09% |
| 106 | AA_composition_R_mean                       | 69. 23% | 99. 37% | 99. 07% |
| 107 | out_local_density_0.4_mean                  | 70. 41% | 99. 40% | 99. 11% |
| 108 | VanDerWaal_distribution_P-0 .75_mean        | 69. 82% | 99. 39% | 99. 10% |
| 109 | out_degree_max                              | 69. 23% | 99. 41% | 99. 12% |
| 110 | polarizability_distribution<br>_N-1.0_mean  | 69. 82% | 99. 38% | 99. 09% |
| 111 | polarizability_distribution<br>_H-0.25_mean | 69. 82% | 99. 37% | 99. 07% |
| 112 | hydrophobicity_distribution<br>_N-1.0_mean  | 69. 23% | 99. 36% | 99. 06% |
| 113 | VanDerWaal_transition_PH_me<br>an           | 69. 23% | 99. 36% | 99. 06% |
| 114 | polarity_distribution_H-0.7<br>5_mean       | 69. 23% | 99. 39% | 99. 09% |

| 115 | in_clustering_mean                               | 69. 82% | 99. 40% | 99. 10% |
|-----|--|---------|---------|---------|
| 116 | polarity_distribution_P-1.0<br>_mean             | 70. 41% | 99. 37% | 99. 08% |
| 117 | secondary_structure_transit<br>ion_NH_mean       | 70. 41% | 99. 37% | 99. 08% |
| 118 | secondary_structure_distrib<br>ution_H-0.25_mean | 71. 01% | 99. 39% | 99. 11% |
| 119 | AA_composition_Y_mean                            | 71. 60% | 99. 37% | 99. 10% |
| 120 | polarizability_distribution<br>_P-0.25_mean      | 71. 01% | 99. 37% | 99. 09% |
| 121 | in_degree_correlation_max                        | 70. 41% | 99. 38% | 99. 09% |
| 122 | polarizability_composition_<br>N_mean            | 70. 41% | 99. 35% | 99. 06% |
| 123 | VanDerWaal_distribution_H-0<br>.75_mean          | 70. 41% | 99. 35% | 99. 06% |

| 124 | solvent_accessibility_distr<br>ibution_H-0.0_mean | 71. 01% | 99. 33% | 99. 05% |
|-----|---|---------|---------|---------|
| 125 | VanDerWaal_distribution_N-0 .5_mean               | 71. 01% | 99. 35% | 99. 07% |
| 126 | polarizability_transition_P<br>N_mean             | 71. 01% | 99. 34% | 99. 06% |
| 127 | secondary_structure_distrib<br>ution_N-0.25_mean  | 71. 01% | 99. 34% | 99. 06% |
| 128 | AA_composition_E_mean                             | 71. 01% | 99. 33% | 99. 05% |
| 129 | out_local_density_0.3_max                         | 71.01%  | 99. 33% | 99. 05% |
| 130 | VanDerWaal_distribution_P-1 .0_mean               | 71. 01% | 99. 33% | 99. 05% |
| 131 | hydrophobicity_distribution<br>_P-1.0_mean        | 71. 01% | 99. 33% | 99. 05% |
| 132 | hydrophobicity_distribution<br>_H-0.75_mean       | 71. 60% | 99. 31% | 99. 04% |

| 133 | secondary_structure_composi<br>tion_P_mean       | 70. 41% | 99. 30% | 99. 01% |
|-----|--|---------|---------|---------|
| 134 | secondary_structure_distrib<br>ution_N-0.75_mean | 70. 41% | 99. 29% | 99. 00% |
| 135 | AA_composition_G_max                             | 70. 41% | 99. 29% | 99. 00% |
| 136 | secondary_structure_distrib<br>ution_H-0.75_mean | 70. 41% | 99. 30% | 99. 02% |
| 137 | in_local_density_0.3_max                         | 70. 41% | 99. 30% | 99. 01% |
| 138 | AA_composition_F_mean                            | 69. 23% | 99. 29% | 98. 99% |
| 139 | VanDerWaal_distribution_N-1 .0_mean              | 69. 82% | 99. 29% | 99. 00% |
| 140 | polarity_transition_PH_mean                      | 69. 82% | 99. 28% | 98. 99% |
| 141 | hydrophobicity_distribution<br>_H-0.25_mean      | 69. 82% | 99. 27% | 98. 98% |

| 142 | secondary_structure_distrib<br>ution_N-0.0_mean        | 69. 82% | 99. 26% | 98. 97% |
|-----|--|---------|---------|---------|
| 143 | graph_size   | 69. 82% | 99. 27% | 98. 97% |
| 144 | <pre>weight_edge_mean(without_mi     ssing_edge)</pre> | 70. 41% | 99. 29% | 99. 00% |
| 145 | polarizability_distribution<br>_P-0.0_mean             | 69. 82% | 99. 28% | 98. 99% |
| 146 | secondary_structure_distrib<br>ution_P-0.5_mean        | 69. 23% | 99. 30% | 99. 00% |
| 147 | secondary_structure_distrib<br>ution_H-1.0_max         | 69. 23% | 99. 30% | 99. 00% |
| 148 | polarity_distribution_H-0.5<br>_mean                   | 69. 23% | 99. 29% | 98. 99% |
| 149 | polarizability_distribution<br>_N-0.0_mean             | 68. 64% | 99. 27% | 98. 96% |
| 150 | polarizability_distribution<br>_N-0.5_mean             | 69. 23% | 99. 25% | 98. 95% |
| 151 | topological_change_0.3_0.4                             | 68. 64% | 99. 23% | 98. 93% |

| 152 | secondary_structure_composi<br>tion_N_mean       | 69. 23% | 99. 23% | 98. 93% |
|-----|--|---------|---------|---------|
| 153 | polarizability_transition_N<br>H_mean            | 69. 23% | 99. 22% | 98. 92% |
| 154 | solvent_accessibility_distr<br>ibution_H-1.0_max | 69. 82% | 99. 19% | 98. 90% |
| 155 | polarity_distribution_N-1.0<br>_mean             | 69. 82% | 99. 18% | 98.89%  |
| 156 | solvent_accessibility_trans<br>ition_HE_mean     | 69. 82% | 99. 18% | 98.89%  |
| 157 | polarizability_distribution<br>_P-0.5_mean       | 69. 82% | 99. 17% | 98.88%  |
| 158 | hydrophobicity_distribution<br>_H-1.0_mean       | 69. 82% | 99. 17% | 98.88%  |
| 159 | polarity_distribution_H-0.0<br>_mean             | 69. 82% | 99. 18% | 98.89%  |
| 160 | secondary_structure_distrib<br>ution_N-1.0_mean  | 69. 23% | 99. 17% | 98. 87% |

| 161 | hydrophobicity_distribution<br>_N-0.75_mean | 69. 23% | 99. 15% | 98. 85% |
|-----|---|---------|---------|---------|
| 162 | out_in_topological_mean                     | 69. 23% | 99. 15% | 98.86%  |
| 163 | AA_composition_I_mean                       | 69. 23% | 99. 14% | 98.85%  |
| 164 | VanDerWaal_distribution_H-1 .0_mean         | 69. 23% | 99. 14% | 98. 85% |
| 165 | hydrophobicity_distribution<br>_P-0.25_mean | 69. 82% | 99. 14% | 98.85%  |
| 166 | AA_composition_M_mean                       | 69. 82% | 99. 13% | 98.84%  |
| 167 | VanDerWaal_distribution_N-0<br>.75_mean     | 69. 82% | 99. 11% | 98. 82% |
| 168 | hydrophobicity_transition_P<br>N_mean       | 69. 82% | 99. 12% | 98. 83% |
| 169 | in_clustering_variance                      | 69. 23% | 99. 14% | 98.85%  |
| 170 | polarity_distribution_N-0.2<br>5_mean       | 68. 05% | 99. 15% | 98. 84% |

| 171 | polarizability_composition_<br>H_mean       | 68. 05% | 99. 14% | 98. 83% |
|-----|---|---------|---------|---------|
| 172 | VanDerWaal_composition_N_me<br>an           | 67. 46% | 99. 14% | 98. 82% |
| 173 | hydrophobicity_transition_N<br>H_max        | 67. 46% | 99. 18% | 98.86%  |
| 174 | AA_composition_Q_max                        | 68. 05% | 99. 18% | 98. 88% |
| 175 | VanDerWaal_distribution_P-0 .0_mean         | 68. 05% | 99. 17% | 98. 86% |
| 176 | out_clustering_variance                     | 67. 46% | 99. 18% | 98.86%  |
| 177 | polarity_distribution_P-0.5<br>_mean        | 67. 46% | 99. 16% | 98.85%  |
| 178 | VanDerWaal_distribution_N-0 .0_mean         | 67. 46% | 99. 17% | 98. 86% |
| 179 | VanDerWaal_distribution_H-0<br>.25_mean     | 67. 46% | 99. 16% | 98. 85% |
| 180 | hydrophobicity_distribution<br>_P-0.75_mean | 68. 05% | 99. 16% | 98. 85% |

| 181 | VanDerWaal_distribution_N-0 .25_mean           | 68. 05% | 99. 17% | 98.86%  |
|-----|--|---------|---------|---------|
| 182 | polarizability_distribution<br>_P-0.75_mean    | 68. 05% | 99. 17% | 98.86%  |
| 183 | secondary_structure_distrib<br>ution_H-0.0_max | 68. 05% | 99. 18% | 98. 87% |
| 184 | polarizability_distribution<br>_H-0.75_mean    | 67. 46% | 99. 17% | 98.86%  |
| 185 | hydrophobicity_distribution<br>_P-0.0_max      | 67. 46% | 99. 16% | 98.85%  |
| 186 | polarizability_composition_<br>P_mean          | 68. 05% | 99. 17% | 98. 86% |
| 187 | in_out_topological_variance                    | 68. 05% | 99. 15% | 98.84%  |
| 188 | secondary_structure_composi<br>tion_H_max      | 67. 46% | 99. 14% | 98.83%  |
| 189 | polarity_transition_PN_mean                    | 67. 46% | 99. 14% | 98.82%  |

| 190 | in_local_density_0.4_max                        | 67. 46% | 99. 14% | 98. 83% |
|-----|---|---------|---------|---------|
| 191 | polarity_distribution_P-0.2<br>5_mean           | 67. 46% | 99. 13% | 98. 82% |
| 192 | polarizability_distribution<br>_H-0.5_mean      | 68. 05% | 99. 12% | 98.82%  |
| 193 | secondary_structure_distrib<br>ution_N-0.75_max | 67. 46% | 99. 15% | 98.84%  |
| 194 | in_in_topological_mean                          | 67. 46% | 99. 17% | 98.85%  |
| 195 | hydrophobicity_distribution<br>_N-0.5_mean      | 67. 46% | 99. 15% | 98. 84% |
| 196 | polarity_distribution_N-0.0<br>_mean            | 66. 86% | 99. 14% | 98. 82% |
| 197 | VanDerWaal_transition_NH_me<br>an               | 66. 86% | 99. 14% | 98. 82% |
| 198 | out_local_density_0.4_max                       | 66. 86% | 99. 14% | 98. 82% |
| 199 | polarity_distribution_P-0.7<br>5_mean           | 66. 86% | 99. 15% | 98. 83% |
| 200 | in_out_topological_mean                         | 66. 27% | 99. 14% | 98.81%  |

| 201 | hydrophobicity_composition_<br>P_mean      | 66. 27% | 99. 14% | 98.81%  |
|-----|--|---------|---------|---------|
| 202 | out_in_topological_variance                | 66. 27% | 99. 15% | 98.82%  |
| 203 | AA_composition_L_max                       | 66. 27% | 99. 14% | 98. 82% |
| 204 | hydrophobicity_distribution<br>_P-0.5_mean | 66. 27% | 99. 14% | 98.82%  |
| 205 | hydrophobicity_composition_<br>N_mean      | 66. 27% | 99. 14% | 98.81%  |
| 206 | polarity_distribution_N-0.7<br>5_mean      | 66. 27% | 99. 13% | 98.80%  |
| 207 | AA_composition_I_max                       | 66. 27% | 99. 14% | 98.81%  |
| 208 | secondary_structure_composi<br>tion_H_mean | 66. 27% | 99. 13% | 98.80%  |
| 209 | VanDerWaal_distribution_P-0 .25_mean       | 66. 27% | 99. 14% | 98.82%  |
| 210 | out_out_topological_mean                   | 66. 27% | 99. 15% | 98.82%  |
| 211 | polarity_transition_PN_max                 | 66. 27% | 99. 15% | 98.82%  |

| 212 | VanDerWaal_composition_H_me<br>an              | 66. 27% | 99. 15% | 98. 82% |
|-----|--|---------|---------|---------|
| 213 | hydrophobicity_distribution<br>_H-0.5_mean     | 66. 27% | 99. 14% | 98. 82% |
| 214 | out_local_density_0.2_mean                     | 66. 27% | 99. 15% | 98. 82% |
| 215 | polarity_transition_NH_mean                    | 66. 27% | 99. 15% | 98.82%  |
| 216 | secondary_structure_composi<br>tion_N_max      | 66. 27% | 99. 14% | 98.81%  |
| 217 | secondary_structure_distrib<br>ution_N-0.5_max | 65. 68% | 99. 14% | 98. 80% |
| 218 | hydrophobicity_distribution<br>_H-0.0_mean     | 65. 68% | 99. 14% | 98.80%  |
| 219 | AA_composition_H_max                           | 65. 68% | 99. 14% | 98. 81% |
| 220 | VanDerWaal_distribution_P-0 .5_mean            | 65. 68% | 99. 12% | 98. 79% |
| 221 | hydrophobicity_distribution<br>_N-0.25_mean    | 65. 09% | 99. 12% | 98.78%  |

| 222 | AA_composition_R_max                             | 65. 09% | 99. 11% | 98.78%  |
|-----|--|---------|---------|---------|
| 223 | first_singular_values                            | 65. 09% | 99. 12% | 98.78%  |
| 224 | AA_composition_W_max                             | 65. 09% | 99. 11% | 98. 78% |
| 225 | hydrophobicity_transition_N<br>H_mean            | 65. 09% | 99. 12% | 98. 79% |
| 226 | polarity_transition_NH_max                       | 65. 09% | 99. 11% | 98. 77% |
| 227 | secondary_structure_distrib<br>ution_H-0.75_max  | 65. 09% | 99. 12% | 98. 79% |
| 228 | polarity_composition_N_mean                      | 65. 09% | 99. 12% | 98. 79% |
| 229 | in_local_density_0.2_mean                        | 65. 09% | 99. 13% | 98. 79% |
| 230 | VanDerWaal_distribution_N-0 .0_max               | 65. 09% | 99. 14% | 98. 80% |
| 231 | solvent_accessibility_distr<br>ibution_H-0.5_max | 65. 09% | 99. 12% | 98. 78% |
| 232 | secondary_structure_transit<br>ion_PH_max        | 65. 68% | 99. 11% | 98. 78% |

| 233 | polarity_composition_H_mean                | 65. 68% | 99. 12% | 98. 79% |
|-----|--|---------|---------|---------|
| 234 | polarity_distribution_N-0.5<br>_mean       | 65. 68% | 99. 12% | 98.79%  |
| 235 | hydrophobicity_distribution<br>_P-0.75_max | 65. 68% | 99. 14% | 98.80%  |
| 236 | AA_composition_S_max                       | 65. 68% | 99. 13% | 98.80%  |
| 237 | AA_composition_E_max                       | 65. 68% | 99. 12% | 98. 79% |
| 238 | VanDerWaal_distribution_P-0<br>.25_max     | 65. 68% | 99. 13% | 98.80%  |
| 239 | polarizability_distribution<br>_N-0.75_max | 65. 68% | 99. 12% | 98. 79% |
| 240 | AA_composition_C_max                       | 65. 68% | 99. 09% | 98.76%  |
| 241 | AA_composition_Y_max                       | 65. 68% | 99. 09% | 98.76%  |
| 242 | AA_composition_T_max                       | 65. 68% | 99. 10% | 98. 77% |
| 243 | VanDerWaal_distribution_H-0 .0_mean        | 65. 68% | 99. 10% | 98.77%  |
| 244 | in_degree_median                           | 65. 68% | 99. 10% | 98.77%  |
| 245 | AA_composition_D_max                       | 65. 68% | 99. 10% | 98.77%  |

| 246 | solvent_accessibility_distr<br>ibution_H-0.75_max | 65. 68% | 99. 09% | 98. 76% |
|-----|---|---------|---------|---------|
| 247 | VanDerWaal_composition_N_ma<br>x                  | 65. 68% | 99. 08% | 98. 75% |
| 248 | hydrophobicity_composition_<br>H_mean             | 66. 27% | 99. 08% | 98. 76% |
| 249 | polarizability_composition_<br>H_max              | 65. 68% | 99. 09% | 98. 76% |
| 250 | VanDerWaal_composition_P_me<br>an                 | 65. 68% | 99. 08% | 98. 75% |
| 251 | secondary_structure_transit ion_PN_max            | 66. 27% | 99. 06% | 98. 73% |
| 252 | VanDerWaal_distribution_H-0<br>.25_max            | 66. 27% | 99. 05% | 98. 72% |
| 253 | AA_composition_K_max                              | 66. 27% | 99. 05% | 98. 72% |
| 254 | VanDerWaal_distribution_P-0 .0_max                | 66. 27% | 99. 05% | 98. 73% |
| 255 | AA_composition_F_max                              | 66. 27% | 99. 05% | 98. 72% |

| 256 | polarizability_distribution<br>_P-0.5_max      | 66. 27% | 99. 04% | 98. 72% |
|-----|--|---------|---------|---------|
| 257 | polarizability_distribution<br>_N-0.25_max     | 66. 27% | 99. 04% | 98. 72% |
| 258 | AA_composition_N_max                           | 66. 27% | 99. 04% | 98. 72% |
| 259 | out_degree_median                              | 66. 27% | 99. 04% | 98. 72% |
| 260 | polarizability_distribution<br>_N-0.0_max      | 66. 27% | 99. 04% | 98.71%  |
| 261 | secondary_structure_distrib<br>ution_H-0.5_max | 66. 27% | 99. 04% | 98. 71% |
| 262 | AA_composition_A_max                           | 66. 27% | 99. 03% | 98.71%  |
| 263 | polarizability_distribution<br>_P-0.75_max     | 65. 68% | 99. 04% | 98. 71% |
| 264 | polarity_composition_P_mean                    | 65. 68% | 99. 04% | 98. 71% |
| 265 | polarizability_distribution<br>_H-0.0_mean     | 65. 68% | 99. 04% | 98. 71% |
| 266 | polarizability_composition_<br>N_max           | 65. 68% | 99. 04% | 98. 71% |

| 267 | polarity_distribution_N-0.2<br>5_max            | 65. 68% | 99. 04% | 98. 71% |
|-----|---|---------|---------|---------|
| 268 | VanDerWaal_transition_PH_ma<br>x                | 65. 68% | 99. 04% | 98. 71% |
| 269 | VanDerWaal_distribution_H-0<br>.5_max           | 65. 68% | 99. 04% | 98. 71% |
| 270 | AA_composition_V_max                            | 65. 68% | 99. 03% | 98. 70% |
| 271 | polarizability_transition_N<br>H_max            | 65. 68% | 99. 03% | 98. 70% |
| 272 | polarity_distribution_H-0.7<br>5_max            | 65. 68% | 99. 04% | 98. 71% |
| 273 | polarity_distribution_P-0.7<br>5_max            | 65. 68% | 99. 04% | 98. 71% |
| 274 | secondary_structure_distrib<br>ution_P-0.25_max | 65. 68% | 99. 03% | 98. 70% |
| 275 | VanDerWaal_distribution_N-0 .5_max              | 65. 68% | 99. 02% | 98. 69% |
| 276 | hydrophobicity_distribution<br>_N-0.5_max       | 65. 68% | 99. 02% | 98. 69% |
| 277 | out_degree_mean                                 | 65. 68% | 99. 02% | 98. 69% |

| 278 | polarizability_transition_P<br>H_max              | 65. 68% | 99. 01% | 98. 68% |
|-----|---|---------|---------|---------|
| 279 | solvent_accessibility_distr<br>ibution_H-0.25_max | 65. 68% | 99. 01% | 98. 68% |
| 280 | solvent_accessibility_trans<br>ition_HE_max       | 65. 68% | 99. 01% | 98. 68% |
| 281 | VanDerWaal_distribution_P-0<br>.75_max            | 65. 68% | 99. 01% | 98. 68% |
| 282 | AA_composition_M_max                              | 65. 68% | 99. 01% | 98. 68% |
| 283 | polarity_distribution_P-0.0<br>_mean              | 65. 68% | 99. 01% | 98. 68% |
| 284 | hydrophobicity_distribution<br>_P-0.5_max         | 65. 68% | 99. 00% | 98. 67% |
| 285 | VanDerWaal_transition_NH_ma<br>x                  | 65. 09% | 99. 00% | 98.66%  |
| 286 | out_local_density_0.1_mean                        | 65. 09% | 98. 99% | 98. 66% |
| 287 | VanDerWaal_transition_PN_ma<br>x                  | 65. 68% | 99. 00% | 98. 67% |

| 288 | hydrophobicity_distribution<br>_H-0.5_max | 65. 68% | 99. 00% | 98. 67% |
|-----|---|---------|---------|---------|
| 289 | secondary_structure_transit<br>ion_NH_max | 65. 68% | 99. 01% | 98. 68% |
| 290 | polarizability_distribution<br>_N-0.5_max | 65. 68% | 99. 00% | 98. 67% |
| 291 | hydrophobicity_composition_<br>P_max      | 65. 68% | 98. 99% | 98. 66% |
| 292 | VanDerWaal_distribution_H-0<br>.75_max    | 65. 68% | 98. 98% | 98. 65% |
| 293 | hydrophobicity_transition_P<br>N_max      | 65. 68% | 98. 99% | 98. 66% |
| 294 | polarizability_distribution<br>_P-0.0_max | 65. 68% | 98. 99% | 98. 66% |
| 295 | VanDerWaal_distribution_N-0<br>.25_max    | 65. 68% | 98. 99% | 98.66%  |
| 296 | polarity_transition_PH_max                | 65. 68% | 98. 98% | 98. 65% |
| 297 | VanDerWaal_distribution_P-0<br>.5_max     | 65. 68% | 98. 98% | 98. 65% |

| 298 | in_local_density_0.1_mean                       | 65. 68% | 98. 98% | 98. 65% |
|-----|---|---------|---------|---------|
| 299 | hydrophobicity_distribution<br>_N-0.25_max      | 65. 09% | 98. 96% | 98.63%  |
| 300 | secondary_structure_distrib<br>ution_N-0.25_max | 65. 09% | 98. 96% | 98. 62% |
| 301 | secondary_structure_composi<br>tion_P_max       | 65. 09% | 98. 96% | 98. 63% |
| 302 | hydrophobicity_distribution<br>_H-0.25_max      | 65. 09% | 98. 96% | 98. 62% |
| 303 | polarity_distribution_H-0.0<br>_max             | 65. 68% | 98. 96% | 98. 63% |
| 304 | secondary_structure_distrib<br>ution_P-0.5_max  | 65. 68% | 98. 97% | 98. 64% |
| 305 | secondary_structure_distrib<br>ution_H-0.25_max | 65. 68% | 98. 96% | 98. 64% |
| 306 | in_degree_mean                                  | 65. 68% | 98. 97% | 98. 64% |
| 307 | VanDerWaal_composition_H_ma<br>x                | 65. 68% | 98. 98% | 98. 65% |

| 308 | topological_change_0.4_0.5                      | 65. 09% | 98. 98% | 98. 64% |
|-----|---|---------|---------|---------|
| 309 | out_out_topological_max                         | 65. 09% | 98. 98% | 98. 64% |
| 310 | polarizability_distribution<br>_H-0.25_max      | 65. 68% | 98. 98% | 98. 65% |
| 311 | polarizability_distribution<br>_P-0.25_max      | 65. 68% | 98. 97% | 98. 64% |
| 312 | polarizability_composition_<br>P_max            | 65. 68% | 98. 96% | 98.64%  |
| 313 | secondary_structure_distrib<br>ution_P-0.75_max | 65. 68% | 98. 98% | 98. 65% |
| 314 | polarity_distribution_H-0.5<br>_max             | 65. 68% | 98. 97% | 98. 64% |
| 315 | polarity_distribution_N-0.7<br>5_max            | 65. 68% | 98. 97% | 98. 64% |
| 316 | hydrophobicity_distribution<br>_N-0.0_max       | 65. 68% | 98. 98% | 98. 65% |
| 317 | VanDerWaal_distribution_N-0 .75_max             | 65. 68% | 98. 98% | 98. 65% |
| 318 | in_in_topological_max                           | 64. 50% | 98. 99% | 98. 65% |

| 319 | hydrophobicity_distribution<br>_P-0.25_max     | 64. 50% | 98. 99% | 98. 65% |
|-----|--|---------|---------|---------|
| 320 | out_local_density_0_mean                       | 64. 50% | 98. 99% | 98.65%  |
| 321 | polarizability_distribution<br>_H-0.5_max      | 64. 50% | 98. 99% | 98.65%  |
| 322 | polarity_composition_H_max                     | 64. 50% | 98. 99% | 98.65%  |
| 323 | VanDerWaal_composition_P_ma<br>x               | 64. 50% | 98. 99% | 98.65%  |
| 324 | polarity_distribution_N-0.5<br>_max            | 64. 50% | 99. 00% | 98.66%  |
| 325 | polarity_distribution_P-0.2<br>5_max           | 64. 50% | 99. 01% | 98.66%  |
| 326 | polarity_distribution_N-0.0<br>_max            | 64. 50% | 99. 01% | 98.66%  |
| 327 | hydrophobicity_transition_P<br>H_max           | 64. 50% | 99. 00% | 98.66%  |
| 328 | hydrophobicity_distribution<br>_N-0.75_max     | 64. 50% | 98. 99% | 98. 65% |
| 329 | secondary_structure_distrib<br>ution_N-0.0_max | 64. 50% | 98. 99% | 98. 65% |

| 330 | polarizability_distribution<br>_H-0.75_max              | 64. 50% | 98. 98% | 98. 64% |
|-----|---|---------|---------|---------|
| 331 | in_local_density_0_mean                                 | 64. 50% | 98. 99% | 98.65%  |
| 332 | AA_composition_P_max                                    | 64. 50% | 98. 98% | 98.64%  |
| 333 | polarity_distribution_P-0.5<br>_max                     | 64. 50% | 98. 98% | 98.64%  |
| 334 | topological_change_0.5_0.6                              | 64. 50% | 98. 96% | 98. 62% |
| 335 | polarity_distribution_P-0.0<br>_max                     | 64. 50% | 98. 96% | 98. 62% |
| 336 | hydrophobicity_distribution<br>_H-0.75_max              | 64. 50% | 98. 97% | 98. 63% |
| 337 | polarity_distribution_H-0.2<br>5_max                    | 64. 50% | 98. 97% | 98. 63% |
| 338 | <pre>weight_edge_variance(with_m     issing_edge)</pre> | 64. 50% | 98. 96% | 98.62%  |
| 339 | hydrophobicity_composition_<br>N_max                    | 64. 50% | 98. 96% | 98. 62% |
| 340 | polarizability_transition_P<br>N_max                    | 64. 50% | 98. 96% | 98. 62% |
| 341 | in_out_topological_max                                  | 64. 50% | 98. 97% | 98.63%  |

| 342 | out_local_density_0.5_max                                  | 64. 50% | 98. 97% | 98. 63% |
|-----|--|---------|---------|---------|
| 343 | <pre>weight_edge_variance(withou     t_missing_edge)</pre> | 64. 50% | 98. 96% | 98. 62% |
| 344 | hydrophobicity_distribution<br>_H-0.0_max                  | 63. 31% | 98. 95% | 98.60%  |
| 345 | in_local_density_0.5_max                                   | 63. 31% | 98. 96% | 98.61%  |
| 346 | polarity_composition_N_max                                 | 63. 31% | 98. 96% | 98.61%  |
| 347 | polarizability_distribution<br>_H-0.0_max                  | 63. 31% | 98. 97% | 98. 62% |
| 348 | VanDerWaal_distribution_H-0 .0_max                         | 63. 31% | 98. 96% | 98.61%  |
| 349 | out_in_topological_max                                     | 63. 31% | 98. 96% | 98.61%  |
| 350 | second_singular_values                                     | 63. 31% | 98. 96% | 98.61%  |
| 351 | graph_density  | 63. 31% | 98. 96% | 98. 61% |
| 352 | third_singular_values                                      | 63. 31% | 98. 96% | 98.61%  |