

Online Supporting Information S4: Two lists obtained by mRMR

(1) MaxRel features list

| Order | Feature name |
|-------|--|
| 1 | out_local_density_0.6_mean |
| 2 | in_local_density_0.6_mean |
| 3 | in_local_density_0.5_mean |
| 4 | out_local_density_0.7_mean |
| 5 | out_local_density_0.5_mean |
| 6 | in_local_density_0.7_mean |
| 7 | in_local_density_0.4_mean |
| 8 | topological_change_0.1_0.2 |
| 9 | out_local_density_0.4_mean |
| 10 | out_local_density_0.8_mean |
| 11 | topological_change_0.2_0.3 |
| 12 | polarity_composition_P_max |
| 13 | hydrophobicity_composition_H_max |
| 14 | in_local_density_0.8_mean |
| 15 | solvent_accessibility_composition_H_max |
| 16 | in_local_density_0.3_mean |
| 17 | weight_edge_mean(with_missing_edge) |
| 18 | weight_edge_mean(without_missing_edge) |
| 19 | out_local_density_0.3_mean |
| 20 | out_local_density_0.7_max |
| 21 | hydrophobicity_transition_NH_max |
| 22 | in_local_density_0.7_max |
| 23 | in_local_density_0.6_max |
| 24 | polarity_transition_PN_max |
| 25 | out_local_density_0.6_max |
| 26 | solvent_accessibility_composition_H_mean |
| 27 | AA_composition_I_max |
| 28 | out_degree_correlation_max |
| 29 | out_local_density_0.9_mean |
| 30 | in_degree_correlation_max |
| 31 | in_degree_variance |
| 32 | AA_composition_C_mean |
| 33 | out_local_density_0.8_max |
| 34 | out_degree_variance |
| 35 | out_clustering_mean |
| 36 | in_local_density_0.9_mean |
| 37 | hydrophobicity_distribution_P-0.75_max |
| 38 | in_clustering_mean |
| 39 | topological_change_0.3_0.4 |
| 40 | topological_change_0.7_0.8 |

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41      in_local_density_0.5_max
42      in_local_density_0.8_max
43      out_local_density_0.5_max
44      AA_composition_S_mean
45      AA_composition_L_mean
46      AA_composition_K_mean
47      hydrophobicity_transition_PH_mean
48      topological_change_0.6_0.7
49      in_clustering_max
50      AA_composition_F_max
51      second_singular_values
52      polarity_transition_PH_mean
53      out_out_topological_variance
54      secondary_structure_composition_P_max
55      out_clustering_max
56      secondary_structure_transition_PH_mean
57      hydrophobicity_transition_PN_mean
58      AA_composition_L_max
59      AA_composition_D_mean
60      secondary_structure_composition_P_mean
61      AA_composition_V_mean
62      polarizability_transition_PH_mean
63      secondary_structure_composition_H_max
64      in_in_topological_variance
65      AA_composition_F_mean
66      polarity_composition_H_mean
67      in_degree_correlation_variance
68      secondary_structure_distribution_H-0.5_max
69      in_local_density_0_mean
70      AA_composition_E_mean
71      secondary_structure_transition_NH_max
72      hydrophobicity_composition_P_mean
73      secondary_structure_transition_NH_mean
74      out_out_topological_max
75      polarity_transition_PN_mean
76      polarity_composition_P_mean
77      solvent_accessibility_transition_HE_mean
78      out_local_density_0_mean
79      solvent_accessibility_transition_HE_max
80      hydrophobicity_composition_H_mean
81      AA_composition_S_max
82      out_degree_correlation_variance
83      hydrophobicity_transition_NH_mean
84      polarity_transition_NH_mean
```

```
85             VanDerWaal_transition_PN_mean
86                     in_degree_max
87             polarity_distribution_H-0.75_max
88                     AA_composition_A_mean
89             secondary_structure_composition_N_max
90                     out_degree_max
91                     AA_composition_W_mean
92             polarity_distribution_P-0.75_max
93                     AA_composition_C_max
94             VanDerWaal_composition_P_max
95                     first_singular_values
96                     in_in_topological_max
97             polarizability_composition_H_mean
98                     VanDerWaal_composition_H_mean
99             secondary_structure_distribution_H-0.75_max
100            secondary_structure_distribution_N-1.0_mean
101            solvent_accessibility_distribution_H-1.0_mean
102            secondary_structure_transition_PN_max
103                     out_local_density_0.1_mean
104                     in_in_topological_mean
105             VanDerWaal_transition_PH_mean
106                     polarity_composition_N_max
107            solvent_accessibility_distribution_H-0.25_mean
108                     out_degree_median
109            solvent_accessibility_distribution_H-0.75_mean
110                     in_local_density_0.1_mean
111            secondary_structure_transition_PN_mean
112                     AA_composition_G_mean
113                     hydrophobicity_composition_P_max
114             hydrophobicity_distribution_H-0.0_mean
115                     VanDerWaal_distribution_H-0.0_mean
116             polarizability_distribution_H-0.0_mean
117                     polarity_distribution_P-0.0_mean
118            solvent_accessibility_distribution_H-0.5_mean
119                     in_degree_median
120             weight_edge_variance(with_missing_edge)
121                     hydrophobicity_composition_N_max
122                     polarity_transition_NH_max
123                     out_out_topological_mean
124             polarizability_transition_PN_mean
125                     third_singular_values
126                     AA_composition_P_max
127             weight_edge_variance(without_missing_edge)
128                     AA_composition_T_mean
```

```
129          AA_composition_M_max
130          AA_composition_P_mean
131          polarity_composition_H_max
132          secondary_structure_distribution_N-0.75_mean
133          secondary_structure_composition_H_mean
134          AA_composition_I_mean
135          hydrophobicity_distribution_N-0.0_mean
136          hydrophobicity_distribution_P-0.5_max
137          solvent_accessibility_distribution_H-0.75_max
138          polarity_composition_N_mean
139          polarizability_composition_N_mean
140          secondary_structure_distribution_H-0.25_max
141          secondary_structure_distribution_P-0.0_mean
142          hydrophobicity_distribution_H-0.25_mean
143          AA_composition_E_max
144          AA_composition_R_mean
145          out_in_topological_mean
146          in_out_topological_mean
147          polarizability_transition_NH_mean
148          out_local_density_0.2_mean
149          VanDerWaal_composition_N_max
150          secondary_structure_distribution_P-0.5_max
151          secondary_structure_composition_N_mean
152          secondary_structure_distribution_P-0.75_max
153          AA_composition_Q_mean
154          in_local_density_0.4_max
155          polarizability_composition_P_mean
156          in_out_topological_max
157          VanDerWaal_composition_P_mean
158          secondary_structure_distribution_N-0.75_max
159          hydrophobicity_distribution_H-0.75_mean
160          hydrophobicity_distribution_H-0.75_max
161          topological_change_0.5_0.6
162          secondary_structure_distribution_N-0.5_mean
163          polarizability_composition_N_max
164          VanDerWaal_transition_NH_mean
165          solvent_accessibility_distribution_H-0.0_mean
166          in_local_density_0.2_mean
167          hydrophobicity_composition_N_mean
168          secondary_structure_distribution_H-0.0_mean
169          secondary_structure_distribution_P-0.75_mean
170          AA_composition_T_max
171          polarity_distribution_P-0.0_max
172          hydrophobicity_distribution_H-0.0_max
```

```
173     polarizability_distribution_H-0.0_max
174         VanDerWaal_distribution_H-0.0_max
175             polarity_distribution_H-0.5_max
176             polarizability_composition_P_max
177     secondary_structure_distribution_H-1.0_mean
178         AA_composition_Y_mean
179         AA_composition_H_mean
180             AA_composition_W_max
181         VanDerWaal_distribution_P-0.0_mean
182             polarity_transition_PN_max
183     secondary_structure_distribution_N-0.25_max
184         polarizability_distribution_H-1.0_mean
185         VanDerWaal_distribution_H-1.0_mean
186             AA_composition_R_max
187     secondary_structure_distribution_N-0.0_max
188         in_local_density_0.9_max
189     secondary_structure_distribution_N-0.5_max
190         polarity_distribution_N-0.0_mean
191         VanDerWaal_distribution_P-0.75_max
192             polarity_distribution_H-0.25_mean
193         polarizability_distribution_P-0.0_mean
194         polarizability_distribution_N-0.0_mean
195             hydrophobicity_transition_PN_max
196             polarity_distribution_H-0.25_max
197     hydrophobicity_distribution_P-0.25_max
198         polarity_distribution_P-0.25_mean
199         polarity_distribution_N-0.75_max
200         polarizability_composition_H_max
201             VanDerWaal_composition_H_max
202             out_local_density_0.9_max
203         polarity_distribution_H-1.0_mean
204         VanDerWaal_transition_NH_max
205             in_out_topological_variance
206             polarity_transition_PH_max
207             polarity_distribution_P-0.5_max
208         polarizability_distribution_N-0.75_mean
209             polarity_distribution_N-0.5_max
210     hydrophobicity_distribution_P-0.25_mean
211         AA_composition_D_max
212         polarizability_distribution_P-0.5_max
213     solvent_accessibility_distribution_H-0.5_max
214         polarity_distribution_H-0.0_max
215             AA_composition_G_max
216             VanDerWaal_distribution_N-0.5_max
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217         out_local_density_0.4_max
218         AA_composition_Q_max
219         VanDerWaal_distribution_N-0.25_mean
220         hydrophobicity_distribution_N-0.75_max
221         polarizability_distribution_N-0.25_mean
222         VanDerWaal_distribution_H-0.75_mean
223         polarizability_distribution_H-0.75_mean
224             polarity_distribution_N-0.0_max
225             polarity_distribution_P-0.75_mean
226         secondary_structure_distribution_H-0.25_mean
227             polarity_distribution_H-0.0_mean
228             hydrophobicity_distribution_P-1.0_mean
229                 out_local_density_0_max
230             polarizability_distribution_P-0.75_max
231                 hydrophobicity_distribution_H-0.5_max
232         secondary_structure_distribution_H-0.5_mean
233         secondary_structure_distribution_H-0.75_mean
234             hydrophobicity_distribution_P-0.75_mean
235             VanDerWaal_distribution_P-0.75_mean
236                 hydrophobicity_transition_PH_max
237             VanDerWaal_distribution_P-0.5_max
238                 AA_composition_K_max
239             hydrophobicity_distribution_P-0.0_mean
240                 polarity_distribution_N-0.25_max
241                     out_local_density_0.1_max
242                     topological_change_0.4_0.5
243                     polarity_distribution_P-1.0_mean
244                     hydrophobicity_distribution_N-0.5_max
245             polarizability_distribution_P-0.25_mean
246                 hydrophobicity_distribution_H-0.25_max
247         secondary_structure_distribution_N-0.25_mean
248             polarity_distribution_H-0.75_mean
249             hydrophobicity_distribution_N-0.0_max
250                 VanDerWaal_composition_N_mean
251                 VanDerWaal_distribution_H-0.5_max
252             polarizability_distribution_H-0.5_max
253             VanDerWaal_distribution_N-0.75_mean
254                 polarity_distribution_P-0.5_mean
255         secondary_structure_distribution_N-0.0_mean
256             out_degree_mean
257                 in_degree_mean
258         secondary_structure_distribution_H-0.0_max
259             AA_composition_V_max
260             VanDerWaal_distribution_N-1.0_mean
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261          AA_composition_Y_max
262          VanDerWaal_distribution_H-0.25_max
263          polarizability_distribution_H-0.25_max
264          VanDerWaal_distribution_N-0.75_max
265          VanDerWaal_distribution_P-0.0_max
266          polarizability_transition_NH_max
267          VanDerWaal_transition_PN_max
268          VanDerWaal_distribution_N-0.0_mean
269          out_in_topological_max
270          solvent_accessibility_distribution_H-0.0_max
271          VanDerWaal_distribution_H-0.75_max
272          polarizability_distribution_H-0.75_max
273          hydrophobicity_distribution_H-1.0_mean
274          secondary_structure_distribution_P-0.5_mean
275          VanDerWaal_distribution_P-0.25_mean
276          hydrophobicity_distribution_N-0.25_mean
277          secondary_structure_distribution_P-0.25_max
278          solvent_accessibility_distribution_H-1.0_max
279          polarity_distribution_P-0.25_max
280          hydrophobicity_distribution_H-0.5_mean
281          AA_composition_N_mean
282          polarizability_distribution_P-0.0_max
283          AA_composition_N_max
284          polarizability_distribution_P-0.75_mean
285          AA_composition_H_max
286          solvent_accessibility_distribution_H-0.25_max
287          out_in_topological_variance
288          secondary_structure_distribution_N-1.0_max
289          polarizability_distribution_N-0.75_max
290          hydrophobicity_distribution_P-0.0_max
291          secondary_structure_distribution_P-0.25_mean
292          VanDerWaal_distribution_N-0.25_max
293          in_degree_correlation_mean
294          polarizability_distribution_N-0.5_max
295          polarizability_distribution_H-0.25_mean
296          VanDerWaal_distribution_H-0.25_mean
297          polarizability_distribution_N-1.0_mean
298          polarity_distribution_N-0.25_mean
299          hydrophobicity_distribution_P-0.5_mean
300          VanDerWaal_distribution_P-0.25_max
301          polarity_distribution_H-0.5_mean
302          AA_composition_M_mean
303          out_degree_correlation_mean
304          VanDerWaal_distribution_H-0.5_mean
```

```
305     polarizability_distribution_H-0.5_mean
306     hydrophobicity_distribution_N-0.25_max
307         VanDerWaal_distribution_N-0.5_mean
308             polarity_distribution_N-0.75_mean
309         polarizability_distribution_P-1.0_max
310         polarizability_distribution_P-0.5_mean
311         hydrophobicity_distribution_N-0.75_mean
312             out_local_density_0.2_max
313         secondary_structure_distribution_P-1.0_mean
314             in_clustering_variance
315         polarizability_distribution_N-0.0_max
316             graph_density
317             AA_composition_A_max
318         VanDerWaal_distribution_N-0.0_max
319         secondary_structure_distribution_H-1.0_max
320             in_local_density_0.3_max
321         polarizability_distribution_N-0.5_mean
322         polarizability_distribution_N-0.25_max
323             secondary_structure_transition_PH_max
324                 polarizability_transition_PH_max
325             hydrophobicity_distribution_H-1.0_max
326                 polarity_distribution_N-1.0_mean
327             VanDerWaal_distribution_P-1.0_mean
328             hydrophobicity_distribution_P-1.0_max
329                 VanDerWaal_distribution_H-1.0_max
330             polarizability_distribution_H-1.0_max
331             polarizability_distribution_P-0.25_max
332                 VanDerWaal_transition_PH_max
333                     out_clustering_variance
334                     in_local_density_0_max
335             hydrophobicity_distribution_N-0.5_mean
336                 VanDerWaal_distribution_P-0.5_mean
337                     in_local_density_0.1_max
338                     polarity_distribution_H-1.0_max
339                     polarity_distribution_N-1.0_max
340                 VanDerWaal_distribution_P-1.0_max
341             hydrophobicity_distribution_N-1.0_max
342                 polarity_distribution_P-1.0_max
343             polarizability_distribution_P-1.0_mean
344             hydrophobicity_distribution_N-1.0_mean
345                 polarity_distribution_N-0.5_mean
346                 VanDerWaal_distribution_N-1.0_max
347                     out_local_density_0.3_max
348                     in_local_density_0.2_max
```

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|-----|--|
| 349 | graph_size |
| 350 | polarizability_distribution_N-1.0_max |
| 351 | secondary_structure_distribution_P-0.0_max |

(2) mRMR features list

| Order | Feature name |
|-------|---|
| 1 | out_local_density_0.6_mean |
| 2 | polarity_composition_P_max |
| 3 | in_local_density_0.7_max |
| 4 | in_local_density_0.5_mean |
| 5 | topological_change_0.6_0.7 |
| 6 | topological_change_0.1_0.2 |
| 7 | in_degree_variance |
| 8 | topological_change_0.7_0.8 |
| 9 | out_local_density_0.8_mean |
| 10 | secondary_structure_distribution_P-1.0_mean |
| 11 | topological_change_0.2_0.3 |
| 12 | in_local_density_0.6_mean |
| 13 | out_degree_variance |
| 14 | secondary_structure_distribution_P-1.0_max |
| 15 | out_local_density_0.5_mean |
| 16 | out_degree_correlation_max |
| 17 | out_local_density_0.7_max |
| 18 | polarizability_distribution_N-1.0_max |
| 19 | in_local_density_0.7_mean |
| 20 | AA_composition_C_mean |
| 21 | in_degree_correlation_variance |
| 22 | secondary_structure_distribution_P-0.0_max |
| 23 | out_local_density_0.7_mean |
| 24 | AA_composition_S_mean |
| 25 | out_degree_correlation_variance |
| 26 | VanDerWaal_distribution_P-1.0_max |
| 27 | polarity_distribution_P-1.0_max |
| 28 | in_local_density_0.8_mean |
| 29 | AA_composition_K_mean |
| 30 | polarity_distribution_H-1.0_max |
| 31 | polarizability_transition_PH_mean |
| 32 | in_clustering_max |
| 33 | hydrophobicity_distribution_N-1.0_max |
| 34 | solvent_accessibility_composition_H_max |
| 35 | out_local_density_0.9_mean |
| 36 | VanDerWaal_distribution_N-1.0_max |
| 37 | secondary_structure_transition_PH_mean |

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38          in_local_density_0.3_mean
39          hydrophobicity_distribution_H-1.0_max
40          in_local_density_0.9_mean
41          out_local_density_0_max
42          solvent_accessibility_distribution_H-1.0_mean
43          in_local_density_0.6_max
44          AA_composition_V_mean
45          VanDerWaal_distribution_H-1.0_max
46          polarizability_distribution_P-1.0_max
47          out_local_density_0.6_max
48          hydrophobicity_distribution_P-1.0_max
49          solvent_accessibility_distribution_H-0.5_mean
50          secondary_structure_distribution_H-0.0_mean
51          in_local_density_0_max
52          solvent_accessibility_composition_H_mean
53          out_degree_correlation_mean
54          out_out_topological_variance
55          AA_composition_W_mean
56          out_local_density_0.8_max
57          out_local_density_0.1_max
58          hydrophobicity_transition_PH_mean
59          polarity_distribution_N-1.0_max
60          in_local_density_0.8_max
61          VanDerWaal_transition_PN_mean
62          out_clustering_max
63          AA_composition_L_mean
64          in_local_density_0.1_max
65          secondary_structure_distribution_P-0.0_mean
66          out_local_density_0.3_mean
67          AA_composition_A_mean
68          AA_composition_H_mean
69          polarizability_distribution_H-1.0_max
70          VanDerWaal_distribution_H-0.5_mean
71          in_in_topological_variance
72          AA_composition_G_mean
73          secondary_structure_distribution_P-0.75_mean
74          in_degree_correlation_mean
75          secondary_structure_distribution_N-1.0_max
76          AA_composition_T_mean
77          polarity_distribution_H-1.0_mean
78          out_local_density_0.9_max
79          secondary_structure_distribution_N-0.5_mean
80          in_local_density_0.9_max
81          in_local_density_0.4_mean
```

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82     secondary_structure_distribution_H-1.0_mean
83         polarizability_distribution_N-0.75_mean
84     solvent_accessibility_distribution_H-0.0_max
85     solvent_accessibility_distribution_H-0.25_mean
86         AA_composition_D_mean
87             out_local_density_0.2_max
88         polarizability_distribution_H-1.0_mean
89         polarizability_distribution_P-1.0_mean
90             in_degree_max
91             weight_edge_mean(with_missing_edge)
92         hydrophobicity_distribution_P-0.0_mean
93     secondary_structure_transition_PN_mean
94         out_clustering_mean
95     polarizability_distribution_N-0.25_mean
96     secondary_structure_distribution_H-0.5_mean
97         AA_composition_Q_mean
98     solvent_accessibility_distribution_H-0.75_mean
99         AA_composition_P_mean
100    secondary_structure_distribution_P-0.25_mean
101        hydrophobicity_composition_H_max
102        polarity_distribution_H-0.25_mean
103        AA_composition_N_mean
104    hydrophobicity_distribution_N-0.0_mean
105        in_local_density_0.2_max
106        AA_composition_R_mean
107        out_local_density_0.4_mean
108    VanDerWaai_distribution_P-0.75_mean
109        out_degree_max
110    polarizability_distribution_N-1.0_mean
111    polarizability_distribution_H-0.25_mean
112    hydrophobicity_distribution_N-1.0_mean
113        VanDerWaai_transition_PH_mean
114        polarity_distribution_H-0.75_mean
115            in_clustering_mean
116        polarity_distribution_P-1.0_mean
117        secondary_structure_transition_NH_mean
118    secondary_structure_distribution_H-0.25_mean
119        AA_composition_Y_mean
120        polarizability_distribution_P-0.25_mean
121            in_degree_correlation_max
122            polarizability_composition_N_mean
123    VanDerWaai_distribution_H-0.75_mean
124    solvent_accessibility_distribution_H-0.0_mean
125        VanDerWaai_distribution_N-0.5_mean
```

```
126          polarizability_transition_PN_mean
127          secondary_structure_distribution_N-0.25_mean
128              AA_composition_E_mean
129              out_local_density_0.3_max
130              VanDerWaal_distribution_P-1.0_mean
131              hydrophobicity_distribution_P-1.0_mean
132              hydrophobicity_distribution_H-0.75_mean
133              secondary_structure_composition_P_mean
134              secondary_structure_distribution_N-0.75_mean
135                  AA_composition_G_max
136              secondary_structure_distribution_H-0.75_mean
137                  in_local_density_0.3_max
138                  AA_composition_F_mean
139                  VanDerWaal_distribution_N-1.0_mean
140                  polarity_transition_PH_mean
141                  hydrophobicity_distribution_H-0.25_mean
142              secondary_structure_distribution_N-0.0_mean
143                  graph_size
144                  weight_edge_mean(without_missing_edge)
145                  polarizability_distribution_P-0.0_mean
146              secondary_structure_distribution_P-0.5_mean
147              secondary_structure_distribution_H-1.0_max
148                  polarity_distribution_H-0.5_mean
149                  polarizability_distribution_N-0.0_mean
150                  polarizability_distribution_N-0.5_mean
151                      topological_change_0.3_0.4
152              secondary_structure_composition_N_mean
153                  polarizability_transition_NH_mean
154              solvent_accessibility_distribution_H-1.0_max
155                  polarity_distribution_N-1.0_mean
156              solvent_accessibility_transition_HE_mean
157                  polarizability_distribution_P-0.5_mean
158                  hydrophobicity_distribution_H-1.0_mean
159                  polarity_distribution_H-0.0_mean
160              secondary_structure_distribution_N-1.0_mean
161                  hydrophobicity_distribution_N-0.75_mean
162                      out_in_topological_mean
163                      AA_composition_I_mean
164                      VanDerWaal_distribution_H-1.0_mean
165                  hydrophobicity_distribution_P-0.25_mean
166                      AA_composition_M_mean
167                      VanDerWaal_distribution_N-0.75_mean
168                  hydrophobicity_transition_PN_mean
169                      in_clustering_variance
```

170 polarity_distribution_N-0.25_mean
171 polarizability_composition_H_mean
172 VanDerWaal_composition_N_mean
173 hydrophobicity_transition_NH_max
174 AA_composition_Q_max
175 VanDerWaal_distribution_P-0.0_mean
176 out_clustering_variance
177 polarity_distribution_P-0.5_mean
178 VanDerWaal_distribution_N-0.0_mean
179 VanDerWaal_distribution_H-0.25_mean
180 hydrophobicity_distribution_P-0.75_mean
181 VanDerWaal_distribution_N-0.25_mean
182 polarizability_distribution_P-0.75_mean
183 secondary_structure_distribution_H-0.0_max
184 polarizability_distribution_H-0.75_mean
185 hydrophobicity_distribution_P-0.0_max
186 polarizability_composition_P_mean
187 in_out_topological_variance
188 secondary_structure_composition_H_max
189 polarity_transition_PN_mean
190 in_local_density_0.4_max
191 polarity_distribution_P-0.25_mean
192 polarizability_distribution_H-0.5_mean
193 secondary_structure_distribution_N-0.75_max
194 in_in_topological_mean
195 hydrophobicity_distribution_N-0.5_mean
196 polarity_distribution_N-0.0_mean
197 VanDerWaal_transition_NH_mean
198 out_local_density_0.4_max
199 polarity_distribution_P-0.75_mean
200 in_out_topological_mean
201 hydrophobicity_composition_P_mean
202 out_in_topological_variance
203 AA_composition_L_max
204 hydrophobicity_distribution_P-0.5_mean
205 hydrophobicity_composition_N_mean
206 polarity_distribution_N-0.75_mean
207 AA_composition_I_max
208 secondary_structure_composition_H_mean
209 VanDerWaal_distribution_P-0.25_mean
210 out_out_topological_mean
211 polarity_transition_PN_max
212 VanDerWaal_composition_H_mean
213 hydrophobicity_distribution_H-0.5_mean

```
214         out_local_density_0.2_mean
215         polarity_transition_NH_mean
216         secondary_structure_composition_N_max
217         secondary_structure_distribution_N-0.5_max
218         hydrophobicity_distribution_H-0.0_mean
219         AA_composition_H_max
220         VanDerWaal_distribution_P-0.5_mean
221         hydrophobicity_distribution_N-0.25_mean
222         AA_composition_R_max
223         first_singular_values
224         AA_composition_W_max
225         hydrophobicity_transition_NH_mean
226         polarity_transition_NH_max
227         secondary_structure_distribution_H-0.75_max
228         polarity_composition_N_mean
229         in_local_density_0.2_mean
230         VanDerWaal_distribution_N-0.0_max
231         solvent_accessibility_distribution_H-0.5_max
232         secondary_structure_transition_PH_max
233         polarity_composition_H_mean
234         polarity_distribution_N-0.5_mean
235         hydrophobicity_distribution_P-0.75_max
236         AA_composition_S_max
237         AA_composition_E_max
238         VanDerWaal_distribution_P-0.25_max
239         polarizability_distribution_N-0.75_max
240         AA_composition_C_max
241         AA_composition_Y_max
242         AA_composition_T_max
243         VanDerWaal_distribution_H-0.0_mean
244         in_degree_median
245         AA_composition_D_max
246         solvent_accessibility_distribution_H-0.75_max
247         VanDerWaal_composition_N_max
248         hydrophobicity_composition_H_mean
249         polarizability_composition_H_max
250         VanDerWaal_composition_P_mean
251         secondary_structure_transition_PN_max
252         VanDerWaal_distribution_H-0.25_max
253         AA_composition_K_max
254         VanDerWaal_distribution_P-0.0_max
255         AA_composition_F_max
256         polarizability_distribution_P-0.5_max
257         polarizability_distribution_N-0.25_max
```

```
258          AA_composition_N_max
259          out_degree_median
260          polarizability_distribution_N-0.0_max
261          secondary_structure_distribution_H-0.5_max
262          AA_composition_A_max
263          polarizability_distribution_P-0.75_max
264          polarity_composition_P_mean
265          polarizability_distribution_H-0.0_mean
266          polarizability_composition_N_max
267          polarity_distribution_N-0.25_max
268          VanDerWaal_transition_PH_max
269          VanDerWaal_distribution_H-0.5_max
270          AA_composition_V_max
271          polarizability_transition_NH_max
272          polarity_distribution_H-0.75_max
273          polarity_distribution_P-0.75_max
274          secondary_structure_distribution_P-0.25_max
275          VanDerWaal_distribution_N-0.5_max
276          hydrophobicity_distribution_N-0.5_max
277          out_degree_mean
278          polarizability_transition_PH_max
279          solvent_accessibility_distribution_H-0.25_max
280          solvent_accessibility_transition_HE_max
281          VanDerWaal_distribution_P-0.75_max
282          AA_composition_M_max
283          polarity_distribution_P-0.0_mean
284          hydrophobicity_distribution_P-0.5_max
285          VanDerWaal_transition_NH_max
286          out_local_density_0.1_mean
287          VanDerWaal_transition_PN_max
288          hydrophobicity_distribution_H-0.5_max
289          secondary_structure_transition_NH_max
290          polarizability_distribution_N-0.5_max
291          hydrophobicity_composition_P_max
292          VanDerWaal_distribution_H-0.75_max
293          hydrophobicity_transition_PN_max
294          polarizability_distribution_P-0.0_max
295          VanDerWaal_distribution_N-0.25_max
296          polarity_transition_PH_max
297          VanDerWaal_distribution_P-0.5_max
298          in_local_density_0.1_mean
299          hydrophobicity_distribution_N-0.25_max
300          secondary_structure_distribution_N-0.25_max
301          secondary_structure_composition_P_max
```

```
302     hydrophobicity_distribution_H-0.25_max
303             polarity_distribution_H-0.0_max
304     secondary_structure_distribution_P-0.5_max
305     secondary_structure_distribution_H-0.25_max
306             in_degree_mean
307             VanDerWaal_composition_H_max
308             topological_change_0.4_0.5
309             out_out_topological_max
310     polarizability_distribution_H-0.25_max
311     polarizability_distribution_P-0.25_max
312             polarizability_composition_P_max
313     secondary_structure_distribution_P-0.75_max
314             polarity_distribution_H-0.5_max
315             polarity_distribution_N-0.75_max
316     hydrophobicity_distribution_N-0.0_max
317             VanDerWaal_distribution_N-0.75_max
318             in_in_topological_max
319     hydrophobicity_distribution_P-0.25_max
320             out_local_density_0_mean
321     polarizability_distribution_H-0.5_max
322             polarity_composition_H_max
323             VanDerWaal_composition_P_max
324             polarity_distribution_N-0.5_max
325             polarity_distribution_P-0.25_max
326             polarity_distribution_N-0.0_max
327             hydrophobicity_transition_PH_max
328     hydrophobicity_distribution_N-0.75_max
329     secondary_structure_distribution_N-0.0_max
330             polarizability_distribution_H-0.75_max
331             in_local_density_0_mean
332             AA_composition_P_max
333             polarity_distribution_P-0.5_max
334             topological_change_0.5_0.6
335             polarity_distribution_P-0.0_max
336     hydrophobicity_distribution_H-0.75_max
337             polarity_distribution_H-0.25_max
338     weight_edge_variance(with_missing_edge)
339             hydrophobicity_composition_N_max
340             polarizability_transition_PN_max
341             in_out_topological_max
342             out_local_density_0.5_max
343     weight_edge_variance(without_missing_edge)
344             hydrophobicity_distribution_H-0.0_max
345             in_local_density_0.5_max
```

```
346          polarity_composition_N_max
347          polarizability_distribution_H-0.0_max
348          VanDerWaal_distribution_H-0.0_max
349          out_in_topological_max
350          second_singular_values
351          graph_density
352          third_singular_values
```