Appendix 1. MRMR Algorithm rank

|  |
| --- |
| mRMR features  Order Fea Name Score |
| 1 9 RctmPI 0.173  2 68 one\_hot8 247.221  3 42 polar\_RASA\_unbound 8.084  4 3 residue\_id 2.608  5 64 one\_hot4 3.380  6 80 LEU 3.721  7 77 GLY 2.938  8 88 TYR 3.047  9 87 TRP 3.137  10 60 conservation 3.121  11 83 PHE 3.174  12 33 minimum\_CX\_bound 3.324  13 89 VAL 3.004  14 81 LYS 3.104  15 73 ASP 3.213  16 24 side\_chain\_mean\_DPX\_bound 3.360  17 71 ARG 3.278  18 78 HIS 3.457  19 72 ASN 3.295  20 66 one\_hot6 3.339  21 79 ILE 3.392  22 25 side\_chain\_standard\_deviation\_DPX\_bound 3.284  23 86 THR 3.214  24 75 GLU 2.903  25 76 GLN 2.989  26 82 MET 2.994  27 84 PRO 2.974  28 85 SER 2.739  29 63 one\_hot3 2.598  30 10 RcsmPI 2.648  31 57 binding\_count 2.383  32 31 side\_chain\_standard\_deviation\_CX\_bound 2.199  33 67 one\_hot7 2.046  34 59 different 2.023  35 17 total\_RASA\_bound 2.010  36 8 RcsASA 1.760  37 58 same 1.631  38 30 side\_chain\_mean\_CX\_bound 1.502  39 23 total\_standard\_deviation\_DPX\_bound 1.345  40 7 RctASA 1.351  41 69 one\_hot9 1.326  42 74 CYS 1.337  43 15 polar\_ASA\_bound 1.287  44 38 no\_polar\_ASA\_unbound 1.147  45 70 ALA 1.124  46 11 RcpASA 1.138  47 20 polar\_RASA\_bound 1.094  48 22 total\_mean\_DPX\_bound 1.054  49 28 total\_mean\_CX\_bound 1.027  50 21 no\_polar\_RASA\_bound 0.930  51 27 minimum\_DPX\_bound 0.901  52 29 total\_standard\_deviation\_CX\_bound 0.865  53 56 hydrophobility\_unbound 0.841  54 19 side\_chain\_RASA\_bound 0.819  55 13 back\_bone\_ASA\_bound 0.792  56 32 maximum\_CX\_bound 0.760  57 55 minimum\_CX\_unbound 0.734  58 16 no\_polar\_ASA\_bound 0.733  59 26 maximum\_DPX\_bound 0.671  60 51 total\_standard\_deviation\_CX\_unbound 0.673  61 12 total\_ASA\_bound 0.566  62 18 back\_bone\_RASA\_bound 0.536  63 52 side\_chain\_mean\_CX\_unbound 0.533  64 14 side\_chain\_ASA\_bound 0.511  65 62 one\_hot2 0.470  66 53 side\_chain\_standard\_deviation\_CX\_unbound 0.425  67 61 one\_hot1 0.404  68 36 side\_chain\_ASA\_unbound 0.381  69 46 side\_chain\_mean\_DPX\_unbound 0.315  70 9 minimum\_DPX\_unbound 0.291  71 45 total\_standard\_deviation\_DPX\_unbound 0.289  72 65 one\_hot5 0.285  73 37 polar\_ASA\_unbound 0.269  74 54 maximum\_CX\_unbound 0.244  75 41 side\_chain\_RASA\_unbound 0.223  76 35 back\_bone\_ASA\_unbound 0.216  77 34 total\_ASA\_unbound 0.199  78 48 maximum\_DPX\_unbound 0.182  79 43 no\_polar\_RASA\_unbound 0.164  80 47 side\_chain\_standard\_deviation\_DPX\_unbound 0.140  81 40 back\_bone\_RASA\_unbound 0.136  82 50 total\_mean\_CX\_unbound 0.131  83 39 total\_RASA\_unbound 0.099 |