

Supporting Information

Characterization of small molecule binding. I. Accurate identification of strong inhibitors in virtual screening

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Table S1. Hydrophobic and hydrophilic atoms in the residues defined according to the functional group it belongs to.

Table S2 the best performance residue group.

Figure S1. Selection of the kernel function and the weight for the positive samples (K_+) in SVM.

Table S1. Hydrophobic and hydrophilic atoms in the residues defined according the functional group it belongs to.

Residue	Hydrophobic atom	Hydrophilic atom
Ala	CA,HA,CB,1HB,2HB,3HB	N,HN,C,O
Cys	CA,HA,CB,1HB,2HB	N,HN,C,O,SG,HG
Asp	CA,HA,CB,1HB,2HB	N,HN,C,O,CG,OD1,OD2
Glu	CA,HA,CB,1HB,2HB,CG,1HG,2HG	N,HN,C,O,CD,OE1,OE2
Phe	CA,HA,CB,1HB,2HB,CG,CD1,HD1,CD2,HD2,CE1,HE1,CE2,HE2,CZ,HZ	N,HN,C,O
Gly	CA,1HA,2HA	N,HN,C,O
His	CA,HA,CB,1HB,2HB,CG,CD2,HD2,CE1,HE1	N,HN,C,O,ND1,HD1(HD),NE2,HE2(HE)
Ile	CA,HA,CB,HB,CG1,1HG1,2HG1,CG2,1HG2,2HG2,3HG2,CD,1HD,2HD,3HD	N,HN,C,O
Lys	CA,HA,CB,1HB,2HB,CG,1HG,2HG,CD,1HD,2HD,CE,1HE,2HE	N,HN,C,O,NZ,1HZ,2HZ,3HZ
Leu	CA,HA,CB,1HB,2HB,CG,HG,CD1,1HD1,2HD1,3HD1,CD2,1HD2,2HD2,3HD2	N,HN,C,O
Met	CA,HA,CB,1HB,2HB,CG,1HG,2HG,CE,1HE,2HE,3HE	N,HN,C,O,SG
Asn	CA,HA,CB,1HB,2HB	N,HN,C,O,CG,OD1,ND2,1HD2,2HD2
Pro	CA,HA,CB,1HB,2HB,CG,1HG,2HG,CD,1HD,2HD	N,C,O
Gln	CA,HA,CB,1HB,2HB,CG,1HG,2HG	N,HN,C,O,CD,OE1,NE2,HE2
Arg	CA,HA,CB,1HB,2HB,CG,1HG,2HG,CD,1HD,2HD	N,HN,C,O,NE,HE,CZ,NH1,NH2,1HH1,2HH1,1HH2,2HH2
Ser	CA,HA,CB,1HB,2HB	N,HN,C,O,OG,HG
Thr	CA,HA,CB,HB,CG2,1HG1,2HG2,3HG2	N,HN,C,O,OG1,HG1
Val	CA,HA,CB,HB,CG1,1HG1,2HG1,3HG1,CG2,1HG2,2HG2,3HG2	N,HN,C,O
Trp	CA,HA,CB,1HB,2HB,CG,CD1,HD1,CD2,CE2,CE3,HE3,CZ2,HZ2,CZ3,HZ3,CH2,HH2	N,HN,C,O,NE1,HE1
Tyr	CA,HA,CB,1HB,2HB,CG,CD1,HD1,CD2,HD2,CE1,HE1,CE2,HE2,CZ	N,HN,C,O,OH,HH

Table S2 the best performance residue group

Chain	Positions
A	8R,9P,23L,26T,32V,47I,48G,51G,54I,81P,82V,86R,87N,90L,97L
B	8R,9P,10L,23L,24L,25D,26T,29D,31T,33L,47I,48G,49G,50I,52G,54I,56V,76L,80T,83N,85I,86G,90L

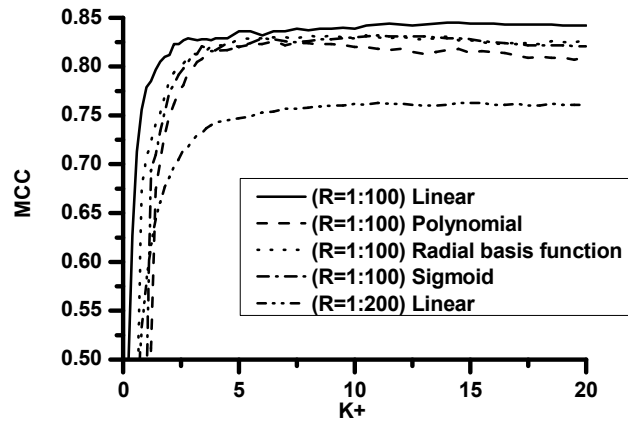


Figure S1. Selection of the kernel function and the weight for the positive samples (K_+) in SVM.