

SUPPLEMENTARY INFORMATION

Table S1. The list of 45 feature vectors used for training.

#	Category	Abbreviation	Feature name
1	Interaction energy	DKE-ele	Docking energy: electrostatic
2	Interaction energy	DKE-hb	Docking energy: hydrogen-bonding
3	Interaction energy	DKE-vdw	Docking energy: van der Waals forces
4	Microenvironment	WCN-c α	WCN: C α atoms in SAV chain
5	Microenvironment	WCN-n	WCN: Nitrogen atoms in SAV chain
6	Microenvironment	WCN-o	WCN: Oxygen atoms in SAV chain
7	Microenvironment	W-H-pol	WCN: <i>H</i> -polar (RKEDQN)
8	Microenvironment	W-H-neu	WCN: <i>H</i> -neutral (GASTPHY)
9	Microenvironment	W-H-hyd	WCN: <i>H</i> -hydrophobic (CVLIMFW)
10	Microenvironment	W-V-sma	WCN: <i>V</i> -small (GASCTPD)
11	Microenvironment	W-V-med	WCN: <i>V</i> -medium (NVEQIL)
12	Microenvironment	W-V-lar	WCN: <i>V</i> -large (MHKFRYW)
13	Microenvironment	W-Z-low	WCN: <i>Z</i> -low polarizability(GASDT)
14	Microenvironment	W-Z-med	WCN: <i>Z</i> - medium polarizability (CPNVEQIL)
15	Microenvironment	W-Z-hig	WCN: <i>Z</i> -high polarizability (KMHFRYW)
16	Microenvironment	W-P-low	WCN: <i>P</i> -low polarity (LIFWCMVY)
17	Microenvironment	W-P-neu	WCN: <i>P</i> -neutral polarity (PATGS)
18	Microenvironment	W-P-hig	WCN: <i>P</i> -high polarity (HQRKNED)
19	Microenvironment	W-F-cha	WCN: <i>F</i> -charged (DEHKR)
20	Microenvironment	W-F-pol	WCN: <i>F</i> -polar (CGNQSTY)
21	Microenvironment	W-F-npo	WCN: <i>F</i> -nonpolar (AFILMPVW)
22	Microenvironment	W-E-aci	WCN: <i>E</i> -acidic (DE)
23	Microenvironment	W-E-bas	WCN: <i>E</i> -basic (HKR)
24	Microenvironment	W-E-aro	WCN: <i>E</i> -aromatic (FWY)
25	Microenvironment	W-E-ami	WCN: <i>E</i> -amide (NQ)
26	Microenvironment	W-E-shy	WCN: <i>E</i> -small hydroxyl (ST)
27	Microenvironment	W-E-sul	WCN: <i>E</i> -sulfur-containing (CM)
28	Microenvironment	W-E-ap1	WCN: <i>E</i> -aliphatic 1 (AGP)
29	Microenvironment	W-E-ap2	WCN: <i>E</i> -aliphatic 2 (ILV)
30	Structure characteristics	BFT	B-factor of SAV

31	Structure characteristics	RSA	Related solvent accessibility
32	Structure characteristics	SSE	Secondary structure elements
33	Structure characteristics	EHB-acc	Energy of backbone H-bond: acceptor
34	Structure characteristics	EHB-don	Energy of Backbone H-bond: donor
35	Sequence conservation	SSI-b62	Substitution index: BLOSUM62
36	Sequence conservation	SSI-p250	Substitution index: PAM250
37	Sequence conservation	SSI-pssm	Substitution index: PSSM
38	Sequence conservation	ETP-sav	Entropy: SAV
39	Sequence conservation	ETP-avg3	Entropy: Average of 3 residues
40	Sequence conservation	ETP-avg5	Entropy: Average of 5 residues
41	Sequence conservation	ETP-avg7	Entropy: Average of 7 residues
42	Sequence conservation	ETP-avg9	Entropy: Average of 9 residues
43	Sequence conservation	ETP-avg11	Entropy: Average of 11 residues
44	Sequence conservation	ETP-avg13	Entropy: Average of 13 residues
45	Sequence conservation	ETP-avg15	Entropy: Average of 15 residues
