Supplementary Text S1: Molecular Descriptor Set

Molecular Descriptor	Description
DCOMPLEX	Atom Level Statistical Potential [1]
GEOMETRIC	Geometric packing potential function
OPUS_PSP1	Orientation-dependent Statistical All-atom Potential Derived from Side-chain Packing term 1 [2]
OPUS_PSP2	Orientation-dependent Statistical All-atom Potential Derived from Side-chain Packing term 2 [2]
OPUS_PSP3	Orientation-dependent Statistical All-atom Potential Derived from Side-chain Packing term 3 [2]
NIP	Normalized interface packing (NIP) [3]
NSc	Normalized Surface complementarity (NSc) score [3]
CHARM_total	CHARMM energy term [4]
CHARM_elec	CHARMM energy term [4]
CHARM_gb	CHARMM energy term [4]
CHARM_sasa	CHARMM energy term [4]
CHARM_gb+sasa	CHARMM energy term [4]
CHARM_vdwaals	CHARMM energy term [4]
ACE19_HYDRophobic	CHARMM19 force field ACE19_COUL - Hydrophobic Burial Term
ACE19_SELF	CHARMM19 force field ACE19_SELF - Electrostatic self-energy (Solvation)
ACE19_SCREENing	CHARMM19 force field ACE19_SCRE - Screening contribution (Solvation)
ACE19_COULomb	CHARMM19 force field ACE19_COUL - Hydrophobic Burial Term
ACE19_SOLVation	CHARMM19 force field ACE19_SOLV - sum of ACE19_SELF+ACE19_SCRE
ACE19_INTERaction	CHARMM19 force field ACE19_INTE - sum of ACE19_SCRE+ACE19_COUL
ACE19_SASL	CHARMM19 force field ACE19_SASL- SASA Solvation energy
PY_fa_atr	Lennard-jones attractive [5]
PY_fa_dun	Internal energy of side-chain rotamers as derived from Dunbrack's statistics based pair term [5]
PY_fa_pair	Favors salt bridges [5]
PY_fa_sol	Lazaridis-jarplus Solvation Energy[5]
PY_hbond_lr_bb	Backbone-backbone H-bonds distant in primary sequence[5]
PY_hbond_sr_bb	Backbone-backbone H-bonds close in primary sequence[5]
PY_fa_intra_rep	Lennard-jones repulsive between atoms in the same residue[5]
PY_fa_rep	Lennard-jones repulsive [5]
PY_hbond_bb_sc	H-bond energy sidechain-backbone[5]
PY_hbond_sc	H-bond energy sidechain-sidechain [5]
PY_pro_close	Proline ring closure energy[5]
FX1_int_BackHbond	Fold-X energy term [6]
FX1_int_SideHbond	Fold-X energy term [6]
FX1_int_Energy_VdW	Fold-X energy term [6]
FX1_int_Electro	Fold-X energy term [6]
FX1_int_Energy_SolvP	Fold-X energy term[6]
FX1_int_Energy_SolvH	Fold-X energy term[6]
FX1_int_Energy_vdwclash	Fold-X energy term[6]
FX1_int_energy_torsion	Fold-X energy term[6]
FX1_int_backbone_vdwclash	Fold-X energy term[6]
FX1_int_Entropy_sidec	Fold-X energy term[6]
FX1_int_Entropy_mainc	Fold-X energy term[6]
FX1_int_water bonds	Fold-X energy term[6]
FX1_int_ helix dipole	Fold-X energy term[6]
FX1_int_loop_entropy	Fold-X energy term[6]
FX1_int_cis_bond	Fold-X energy term[6]
FX1_int_disulfide	Fold-X energy term[6]
FX1_int_kn electrostatic	Fold-X energy term[6]
FX1_int_partial covalent interactions	Fold-X energy term[6]
FX1_int_Energy_Ionisation	Fold-X energy term[6]
FX1_int_Entropy Complex	Fold-X energy term[6]
FX2_BackHbond	Fold-X energy term[6]
FX2_SideHbond	Fold-X energy term[6]
FX2_Energy_VdW	Fold-X energy term[6]
FX2_Electro	Fold-X energy term[6]
FX2_Energy_SolvP	Fold-X energy term[6]
FX2_Energy_SolvH	Fold-X energy term[6]
FX2_Energy_vdwclash	Fold-X energy term[6]
FX2_energy_torsion	Fold-X energy term[6]
FX2_backbone_vdwclash	Fold-X energy term[6]
FX2_Entropy_sidec	Fold-X energy term[6]
FX2_Entropy_mainc	Fold-X energy term[6]
FX2_water bonds	Fold-X energy term[6]
FX2_ helix dipole	Fold-X energy term[6]
FX2_loop_entropy	Fold-X energy term[6]
FX2_cis_bond	Fold-X energy term[6]
FX2_disulfide	Fold-X energy term[6]
FX2_kn electrostatic	Fold-X energy term[6]
FX2_partial covalent interactions	Fold-X energy term[6]
FX2_Energy_Ionisation	Fold-X energy term[6]
FX2_Entropy Complex	Fold-X energy term[6]
DFIRE	Atom Based Statistical Potential [7]
CP_BFKV	Residue Level Statistical Potential [8]
CP_BL	Residue Level Statistical Potential [9]

CP_BT	Residue Level Statistical Potential [10]
CP_GKS	Residue Level Statistical Potential [11]
CP_HLPL	Residue Level Statistical Potential [12]
CP_MJPL	Residue Level Statistical Potential [12]
CP_MJ3h	Residue Level Statistical Potential [13]
CP_MJ2h	Residue Level Statistical Potential [14]
CP_MJ1	Residue Level Statistical Potential [15]
CP_MJ2	Residue Level Statistical Potential [14]
CP_MSBM	Residue Level Statistical Potential [16]
CP_MS	Residue Level Statistical Potential [17]
CP_Qa	Residue Level Statistical Potential [18]
CP_Qm	Residue Level Statistical Potential [18]
CP_Qp	Residue Level Statistical Potential [18]
CP_RO	Residue Level Statistical Potential [19]
CP_SKOb	Residue Level Statistical Potential [20]
CP_SKOa	Residue Level Statistical Potential [20]
CP_SJKG	Residue Level Statistical Potential [21]
CP_TD	Residue Level Statistical Potential [22]
CP_TEl	Residue Level Statistical Potential [23]
CP_TEs	Residue Level Statistical Potential [23]
CP_TS	Residue Level Statistical Potential [24]
CP_VD	Residue Level Statistical Potential
AP_DARS	Statistical Potential [25]
AP_URS	Statistical Potential [25]
AP_MPS	Statistical Potential [25]
DDFIRE	dDFIRE Statistical Potential [26]
AP_DOPE	Standard Dope Potential [27]
AP_DOPE_HR	High-Resolution Dope Potential [27]
CP_RMFCEN1	6 bin distance-dependent centroid-centroid potential [28]
CP_RMFCEN2	7 bin distance-dependent centroid-centroid potential [28]
CP_RMFCA	Alpha-Carbon Potential [29]
CP_SKOIP	Statistical Intermolecular Contact Potential [30]
CP_TB	Docking Contact Potential [31]
CP_TSC	2-Bin Docking Potential [32]
AP_T1	Two-step docking atomistic potential [32]
AP_T2	Two-step docking atomistic potential [32]

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