Material for the Protein Ligandability Recognition task

Task Predict ligandability of the points on the protein's surface and their distances to the closest ligand

Objects Points on protein surface

Target values class, ligand_distance

Feature vector

feature	type*	description
protein_id	a	protein's id
hydrophobic	a	hydrophobic residues
hydrophilic	a	hydrophilic
hydrophatyIndex	a	side-chain hydrophaty index
aliphatic	a	aliphatic residues
aromatic	a	aromatic residues
sulfur	a	residues containing sulfur
hydroxyl	a	hydroxyl group containing residues
basic	a	basic residues
acidic	a	acidic residues
amide	a	amide group containing residues
posCharge	a	positively charged residues
negCharge	a	negatively charged residues
hBondDonor	a	H-bond donor containing residues
hBondAcceptor	a	H-bond acceptor containing residues
hBondDonorAcceptor	a	residues that have H-bond donor AND acceptor
polar	a	polar residues
ionizable	a	ionizable residues
vsAromatic	a	VolSite atomic level features
vsCation	a	
vsAnion	a	
vsHydrophobic	a	
vsAcceptor	a	
vsDonor	a	
atomicHydrophobicity	a	hydrophobicity scale
apRawValids	a	ligand binding propensity for biologically valid ligands
apRawInvalids	a	ligand binding propensity for biologically invalid ligands
bfactor	a	B-factor number of the atom
atoms	c	absolute number of protein exposed atoms in the neighbourhood
atomDensity	c	number of protein exposed atoms in the neighbourhood
atomC	c	number of carbon atoms in the neighbourhood
atomO	c	number of oxygen in the neighbourhood
atomN	c	number of nitrogen in the neighbourhood
hDonorAtoms	c	number of H-bond donor atoms in the neighbourhood
hAcceptorAtoms	c	number of H-bond acceptor atoms in the neighbourhood
protrusion	c	protein surface protrusion
class		0/1 ligandability
ligand_distance		distance between the given example and the closest ligand measured in angstroms (= 10^10 m)

* a – atom, c – atom neighbourhood