QikProp Descriptors and Properties

For each successfully processed molecule, QikProp produces the following descriptors and properties. Those that are not predicted in fast mode are marked with a dagger (†). Those whose values differ between fast and normal mode are marked with a double dagger (‡). Additional information on many of these properties can be found in the *QikProp User Manual*.

Table 2.1. QikProp properties and descriptors. Range is for 95% of known drugs.

Property or Descriptor	Description	Range or recommended values
molecule name	Molecule name taken from the title line in the input structure file. If the title line is blank, the input file name is used.	
#stars	Number of property or descriptor values that fall outside the 95% range of similar values for known drugs. Outlying descriptors and predicted properties are denoted with asterisks (*) in the `.out` file. A large number of stars suggests that a molecule is less drug-like than molecules with few stars. The following properties and descriptors are included in the determination of #stars: MW, dipole, IP, EA, SASA, FOSA, FISA, PISA, WPSA, PSA, volume, #rotor, donorHB, accptHB, glob, QPpolrz, QPlogPC16, QPlogPoct, QPlogPw, QPlogPo/w, logS, QPLogKhsa, QPlogBB, #metabol	0 – 5
#amine	Number of non-conjugated amine groups.	0 – 1
#amidine	Number of amidine and guanidine groups.	0
#acid	Number of carboxylic acid groups.	0 – 1
#amide	Number of non-conjugated amide groups.	0 – 1
#rotor	Number of non-trivial (not CX3), non-hindered (not alkene, amide, small ring) rotatable bonds.	0 – 15
#rtvFG	Number of reactive functional groups; the specific groups are listed in the *jobname* `.out` file. The presence of these groups can lead to false positives in HTS assays and to decomposition, reactivity, or toxicity problems *in vivo*. See Appendix A of the *QikProp User Manual* for a complete list.	0 – 2
CNS	Predicted central nervous system activity on a –2 (inactive) to +2 (active) scale.	–2 to +2
mol_MW	Molecular weight of the molecule.	130.0 – 725.0
dipole†	Computed dipole moment of the molecule.	1.0 – 12.5
SASA	Total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius.	300.0 – 1000.0
FOSA	Hydrophobic component of the SASA (saturated carbon and attached hydrogen).	0.0 – 750.0
FISA	Hydrophilic component of the SASA (SASA on N, O, and H on heteroatoms).	7.0 – 330.0
PISA	π (carbon and attached hydrogen) component of the SASA.	0.0 – 450.0
WPSA	Weakly polar component of the SASA (halogens, P, and S).	0.0 – 175.0
volume	Total solvent-accessible volume in cubic angstroms using a probe with a 1.4 Å radius.	500.0 – 2000.0
donorHB	Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer.	0.0 – 6.0
accptHB	Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer.	2.0 – 20.0

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Property or Descriptor	Description	Range or recommended values
dip^2/V†	Square of the dipole moment divided by the molecular volume. This is the key term in the Kirkwood-Onsager equation for the free energy of solvation of a dipole with volume V.	0.0 – 0.13
ACxDN^.5/SA	Index of cohesive interaction in solids. This term represents the relationship $(accptHB(\sqrt{donorHB}))/(SA)$; see *Bioorg. Med. Chem. Lett.* **2000**, *10*, 1155.	0.0 – 0.05
glob	Globularity descriptor, $(4\pi r^2)/(SASA)$, where *r* is the radius of a sphere with a volume equal to the molecular volume. Globularity is 1.0 for a spherical molecule.	0.75 – 0.95
QPpolrz	Predicted polarizability in cubic angstroms.	13.0 – 70.0
QPlogPC16	Predicted hexadecane/gas partition coefficient.	4.0 – 18.0
QPlogPoct‡	Predicted octanol/gas partition coefficient.	8.0 – 35.0
QPlogPw	Predicted water/gas partition coefficient.	4.0 – 45.0
QPlogPo/w	Predicted octanol/water partition coefficient.	–2.0 – 6.5
QPlogS	Predicted aqueous solubility, log S. S in mol dm^{-3} is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid.	–6.5 – 0.5
CIQPlogS	Conformation-independent predicted aqueous solubility, log S. S in mol dm^{-3} is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid.	–6.5 – 0.5
QPlogHERG	Predicted IC_{50} value for blockage of HERG K^+ channels.	concern below –5
QPPCaco	Predicted apparent Caco-2 cell permeability in nm/sec. Caco-2 cells are a model for the gut-blood barrier. QikProp predictions are for non-active transport.	<25 poor, >500 great
QPlogBB	Predicted brain/blood partition coefficient. Note: QikProp predictions are for orally delivered drugs so, for example, dopamine and serotonin are CNS negative because they are too polar to cross the blood-brain barrier	–3.0 – 1.2
QPPMDCK	Predicted apparent MDCK cell permeability in nm/sec. MDCK cells are considered to be a good mimic for the blood-brain barrier. QikProp predictions are for non-active transport.	<25 poor, >500 great
QPlogKp	Predicted skin permeability, log K_p.	–8.0 – –1.0
IP(ev)†	PM3 calculated ionization potential.	7.9 – 10.5
EA(eV)†	PM3 calculated electron affinity.	–0.9 – 1.7
#metab‡	Number of likely metabolic reactions. See Appendix A of the *QikProp User Manual* for a complete list of reactions.	1 – 8
QPlogKhsa	Prediction of binding to human serum albumin.	–1.5 – 1.5
HumanOralAbsorption	Predicted qualitative human oral absorption: 1, 2, or 3 for low, medium, or high. The text version is reported in the output. The assessment uses a knowledge-based set of rules, including checking for suitable values of PercentHumanOralAbsorption, number of metabolites, number of rotatable bonds, logP, solubility and cell permeability.	
PercentHumanOralAbsorption	Predicted human oral absorption on 0 to 100% scale.The prediction is based on a quantitative multiple linear regression model. This property usually correlates well with HumanOralAbsorption, as both measure the same property.	>80% is high <25% is poor
SAFluorine	Solvent-accessible surface area of fluorine atoms.	0.0 – 100.0
SAamideO	Solvent-accessible surface area of amide oxygen atoms.	0.0 – 35.0
PSA	Van der Waals surface area of polar nitrogen and oxygen atoms.	7.0 – 200.0
#NandO	Number of nitrogen and oxygen atoms.	2 – 15

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Property or Descriptor	Description	Range or recommended values
RuleOfFive	Number of violations of Lipinski's rule of five. The rules are: mol_MW < 500, QPlogPo/w < 5, donorHB ≤ 5, accptHB ≤ 10. Compunds that satisfy these rules are considered drug-like. (The "five" refers to the limits, which are multiples of 5.)	maximum is 4
RuleOfThree	Number of violations of Jorgensen's rule of three. The three rules are: , QPlogS > -5.7, QP PCaco > 22 nm/s, # Primary Metabolites < 7. Compounds with fewer (and preferably no) violations of these rules are more likely to be orally available.	maximum is 3
#ringatoms	Number of atoms in rings.	
#in34	Number of atoms in 3- or 4-membered rings.	
#in56	Number of atoms in 5- or 6-membered rings.	
#noncon	number of ring atoms not able to form conjugated aromatic systems (e.g. sp^3 C).	
#nonHatm	Number of heavy atoms (nonhydrogen atoms).	
Jm	Predicted maximum transdermal transport rate, $K_p \times MW \times S$ (μg cm^{-2} hr^{-1}). K_p and S are obtained from the aqueous solubility and skin permeability, QPlogKp and QPlogS. This property is only written to the output file: it is not used in any other calculations.	