APPENDIX D: Descriptors (Optional)

ADMET Predictor generates 356 molecular descriptors from the 3D structure inputs and 325 descriptors from 2D inputs (04/16/2008). Some of these descriptors are used in the mathematical models for the predicted ADMET properties. Descriptor display is contingent upon the ADMET Modeler Module license. The complete list of descriptors is presented in several tables below, with a brief explanation of each descriptor.

Table 1. Simple Constitutional Descriptors:

Formula	Molecular Formula
MWt	Molecular Weight (g/mol)
MolVol	Liquid molal volume (cm^3/mol) at the normal boiling point is based on Schroeder's method
VMcGowan	Mc Gowan's characteristic volume
N_Atoms	Number of atoms
N_Carbon	Number of carbons
N_Ntrgen	Number of nitrogens
N_Oxygen	Number of oxygens
N_Phsphr	Number of phosphorus atoms
N_Sulfur	Number of sulfurs
N_Fluorn	Number of fluorines
N_Chlorn	Number of chlorines
N_Bromin	Number of bromines
N_Iodine	Number of iodines
N_Halogen	Number of halogen atoms
N_Nonorgn	Number of "non-organic" atoms (i.e., atoms other than C,N,O,S,P,halogens)
N_Metal	Number of metallic element atoms
N_Bonds	Number of bonds
N_FrRotB	Number of freely rotatable bonds, terminal bonds excluded. At least one bonded atom must be sp3-hybridized.
F_SgleB	Single bonds as fraction of total bonds.
F_DbleB	Double bonds as fraction of total bonds.
F_TpleB	Triple bonds as fraction of total bonds.
F_AromB	Aromatic bonds as fraction of total bonds.
F_AFRBWF	Average value of the freely rotatable bond weight factor. The FRBW factor is defined as the minimal atom count fraction per bond.
N_Rings	Number of rings
N_AromR	Number of aromatic rings
N_AlipR	Number of aliphatic rings
N_Pisyms	Number of distinct π systems, excluding lone pairs
N_IsolLP	Number of isolated lone electron pairs
N_Kekule	Number of Kekule structures per molecule
Herndon	Herndon resonance energy
AlHdrxl_-OH	Number of aliphatic hydroxyl groups
ArHdrxl_-OH	Number of aromatic hydroxyl groups
Carbonyl_C=O	Number of carbonyl (ketone or aldehyde) groups
Ether___-O-	Number of ether groups

PriAmine_-NH2	Number of primary amines
PriAmAli_-NH2	Number of primary amines attached to aliphatic carbon
PriAmAro_-NH2	Number of primary amines attached to aromatic carbon
SecAmine_>NH	Number of primary and aliphatic N secondary amines
TerAmine_>N-	Number of tertiary amine groups
QuaAmine_>[N+]<	Number of quaternary amine groups
ArNitrog_=N-	Number of aromatic nitrogens
Imine___=N-	Number of Imine groups
Nitrile_C#N	Number of Nitrile groups
Isocynd_[N+]#[C-]	Number of Isocyanide groups
Thiol___-SH	Number of Thiol groups
ThioCrbl_C=S	Number of Thiocarbonyl groups
Sulfide_-S-	Number of Sulfide groups
Slfonium_>[S+]-	Number of Sulfonium groups
Phsphine_>P-	Number of Phosphine groups
HydxlAmn_>N-O-	Number of Hydroxyamine groups
Oxime___=N-O-	Number of Oxime groups
Nitroso_-N=O	Number of Nitroso groups
Hdrzine_>N-N<	Number of Hydrazine groups
Hdrzone_=N-N<	Number of Hydrazone groups
Azo_____-N=N-	Number of Azo groups
Diazo___-[N+]#N	Number of Diazo groups
ThioAmin_>N-S-	Number of Thioamine groups
Disulfde_-S-S-	Number of Disulfide groups
Sulfoxde_>S=O	Number of Sulfoxide groups
Thioxime_=N-S-	Number of Thioxime groups
Nitro___-NO2	Number of Nitro groups
Nitrite_-O-N=O	Number of Nitrite groups
Ntrosam_>N-N=O	Number of Nitrosamine groups
Azoxy___-N(=O)=N-	Number of Azoxy groups
Azide___-N=N#N	Number of Azide groups
Sulfone_>S(=O)=O	Number of Sulfone groups
Sulfinat_S(=O)O-	Number of Sulfinate groups
Phsporat_P(=O)O-	Number of Phosphorate groups
Triazo__-N-N-N-	Number of Triazo groups
Oxadiazo_-N-O-N-	Number of Oxadiazo groups
Thiadiaz_-N-S-N-	Number of Thiadiazo groups
Triazene_-N=N-N-	Number of Triazene groups
Nitrate_-O-NO2	Number of Nitrate groups
NNitro__>N-NO2	Number of N-connected nitro groups
Sulfonat_-SO3-	Number of Sulfonate groups
Sulfite_-SO3<	Number of Sulfite groups
Sulfonmd_-SO2-N<	Number of Sulfonamide groups
PriSlfmd_-SO2-NH2	Number of Primary Sulfonamide groups
Phsponat_-PO3<	Number of Phosphonate groups
Sphspnat_-SPO2<	Number of Thiolophosphonate groups
Phspite_-OPO2<	Number of Phosphite groups
Tetrazo_-NNNN-	Number of Tetrazo groups
Oxdzoxde_-N(=O)ON-	Number of Oxadiazooxide groups

NOHydxam_-N(N=O)OH	Number of N-nitrosohydroxylamine groups
Sulfamid_>NSO2N<	Number of Sulfamide groups
Sulfate_-OSO3	Number of Sulfate groups
ThioSulf_-SSO3	Number of Thiosulfate groups
Phspate_O=PO3<-	Number of Phosphate groups
PhspatS_O=PS(k)O(3-k)<-	Number of ThioloPhosphate O=P(X)(X)X groups (X = S,O)
Sphspat_S=PO3<-	Number of ThioPhosphate groups
SphspatS_S=PS(k)O(3-k)<-	Number of ThioThioloPhosphate S=P(X)(X)X groups (X = S,O)
PhspatN_O=PN(n)O(3-n)<<<	Number of Phosphamide O=P(X)(X)X groups (X = N,O)
SphspatN_S=PN(n)O(3-n)<<<	Number of ThioPhosphamide S=P(X)(X)X groups (X = N,O)
PhsptSN_O=PS(k)N(n)O(3-n-k)<<	Number of ThioloPhosphamide O=P(X)(X)X groups (X = N,O,S)
SPhsptSN_S=PS(k)N(n)O(3-n-k)<<	Number of ThioThioloPhosphamide S=P(X)(X)X groups (X = N,O,S)
Diphspat_O=PO2-O-PO2=O	Number of Diphosphate groups
Triphspt_O=PO2-O-PO(=O)-OPO2=O	Number of Triphosphate groups
AlCbxyl_-COOH	Number of Aliphatic Carboxyl groups
ArCbxyl_-COOH	Number of Aromatic Carboxyl groups
Ester___C(=O)OC	Number of Ester groups
Amide___C(=O)N<	Number of Amide groups
Thioamd_C(=S)N<	Number of Thioamide groups
Amidine_C(=N-)N<	Number of Amidine groups
Isocyant_-N=C=O	Number of Isocyanate groups
Thiocynt_-S-C#N	Number of Thiocyanate groups
Isothcnt_-N=C=S	Number of Isothiocyanate groups
Urea____>NC(=O)N<	Number of Urea groups
Carbmte_>NC(=O)O-	Number of Carbamate groups
Guandne_>NC(=N-)N<	Number of Guanidine groups
Imide___O=C(N-)C=O	Number of Imide groups
Barbitur_C1C(=O)NC(=O)NC1=O	Number of Barbiturate groups
Unknown_	Number of detected but unassigned functional groups

Table 2. Topological Indices:

X0	Zeroth Order Simple Connectivity Index
X1	First Order Simple Connectivity Index
X2	Second Order Simple Connectivity Index
Kappa1	First Order Simple Kier-Hall shape descriptor
Kappa2	Second Order Simple Kier-Hall shape descriptor
Kappa3	Third Order Simple Kier-Hall shape descriptor
T_Rgrav	Topological equivalent of RgGrav_3D
T_Rgeom	Topological equivalent of RgGeom_3D
T_Radmax	Topological equivalent of RadMax_3D
T_Dipole	Topological equivalent of Dipole_3D
T_Grav3	Topological equivalent of Grav3_3D
T_RDmtr	Relative topological diameter: maximal topological distance divided by the number of atoms
T_PSA	Topological polar surface area, as defined by P. Ertl, et al.
Wiener	Classical Wiener index of the hydrogen-suppressed molecular graph

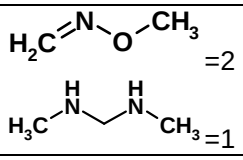
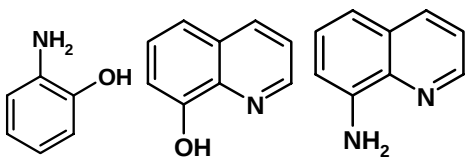
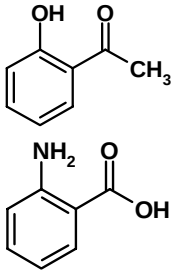
Blbn_J	Balaban distance connectivity index J of the hydrogen-suppressed molecular graph
Blbn_MSD	Balaban mean square distance index of the hydrogen-suppressed molecular graph

Table 3: Atom-type Electropological State Indices:

SsCH3	Atom-type E-state index for -CH3 groups
SdCH2	Atom-type E-state index for =CH2 groups
SssCH2	Atom-type E-state index for -CH2- groups
StCH	Atom-type E-state index for #CH groups
SdsCH	Atom-type E-state index for =CH- groups
SaaCH	Atom-type E-state index for aCHa groups
SsssCH	Atom-type E-state index for >CH- groups
SddC	Atom-type E-state index for =C= groups
StsC	Atom-type E-state index for #C- groups
SdssC	Atom-type E-state index for =C< groups
SaasC	Atom-type E-state index for -Caa groups
SaadC	Atom-type E-state index for =Caa groups (e.g., C=O in theophylline)
SaaaC	Atom-type E-state index for aCaa groups
SssssC	Atom-type E-state index for >C< groups
SsNH2	Atom-type E-state index for -NH2 groups
SdNH	Atom-type E-state index for =NH groups
SssNH	Atom-type E-state index for -NH- groups
SaaNH	Atom-type E-state index for aNHa groups
StN	Atom-type E-state index for #N groups
SdsN	Atom-type E-state index for =N- groups
SdssN	Atom-type E-state index for =N< groups (secondary N-oxide)
SdsssN	Atom-type E-state index for =N<- groups (tertiary N-oxide)
StsN	Atom-type E-state index for -N+# groups (diazonium)
StdN	Atom-type E-state index for #N= groups (azide)
SaaN	Atom-type E-state index for aNa groups
SsssN	Atom-type E-state index for >N- groups
SddsN	Atom-type E-state index for -N== groups (nitro)
SaasN	Atom-type E-state index for aaN- groups (e.g., substituted imidazole)
SaadN	Atom-type E-state index for aaN= groups (aromatic N-oxide)
SaaaN	Atom-type E-state index for aaNa groups (N-fused rings)
SssssN	Atom-type E-state index for >N+< groups (onium)
SsOH	Atom-type E-state index for -OH groups
SdO	Atom-type E-state index for =O groups
SssO	Atom-type E-state index for -O- groups
SsO-	Atom-type E-state index for coordinated O- groups
SaaO	Atom-type E-state index for aOa groups
SsPH2	Atom-type E-state index for -PH2 groups
SssPH	Atom-type E-state index for -PH- groups
SdssPH	Atom-type E-state index for =PH< groups (phosphinate)
SsssP	Atom-type E-state index for >P- groups
SdsssP	Atom-type E-state index for ->P= groups

SsssP	Atom-type E-state index for >P+< groups (phosphonium)
SssssP	Atom-type E-state index for ->P< groups
SsSH	Atom-type E-state index for -SH groups
SdS	Atom-type E-state index for =S groups
SssS	Atom-type E-state index for -S- groups
SsssS	Atom-type E-state index for -S+< groups (sulfonium)
SaaS	Atom-type E-state index for aSa groups
SdssS	Atom-type E-state index for >S= groups (sulfone)
SddssS	Atom-type E-state index for >S== groups (sulfate)
SsssssS	Atom-type E-state index for ->S<- groups
SsF	Atom-type E-state index for -F groups
SsCl	Atom-type E-state index for -Cl groups
SsBr	Atom-type E-state index for -Br groups
SsI	Atom-type E-state index for -I groups
SHsOH	Atom-type hydrogen E-state index for -OH groups
SHdNH	Atom-type hydrogen E-state index for =NH groups
SHsSH	Atom-type hydrogen E-state index for -SH groups
SHsNH2	Atom-type hydrogen E-state index for -NH2 groups
SHssNH	Atom-type hydrogen E-state index for -NH- groups
SHtCH	Atom-type hydrogen E-state index for #CH groups
SHCH_321	Atom-type hydrogen E-state index for -CH3, -CH2- and >CH- groups (saturated aliphatic carbon)
SHdCH2	Atom-type hydrogen E-state index for =CH2 groups
SHdsCH	Atom-type hydrogen E-state index for =CH- groups
SHaaCH	Atom-type hydrogen E-state index for aCHa groups (aromatic carbons)
S_unknown	Counts the number of unrecognized E-state atom types. Please examine relevant molecules and inform Simulations Plus if you suspect this is a software bug.

Table 4. Moriguchi Descriptors for MlogP:

Parameter	Description	Example
M_CX	Summation of numbers of carbon and halogen atoms weighted by C:1.0, F:0.5, Cl:1.0, Br:1.5, and I:2.0.	
M_NO	Total number of N and O atoms	
M_PRX	Proximity effect of N & O; where X-Y:2.0, X-A-Y:1.0 (X,Y can be N or O and A can be C,S, or P) with a correction (-1) for carboxamide/sulfonamide.	 =2 =1
M_UB	Total number of unsaturated bonds except those in NO_2	 =3
M_HB	Number of intramolecular hydrogen bonds as *ortho* –OH and –C(=O)-R, or –OH and $–NH_2$, or $–NH_2$ and –COOH, or 8-OH/NH_2 in quinolines, *etc.*	 

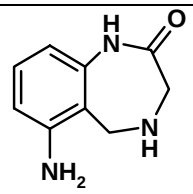
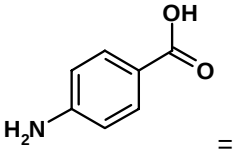
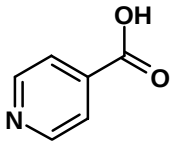
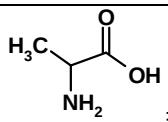
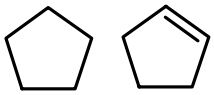
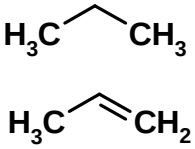
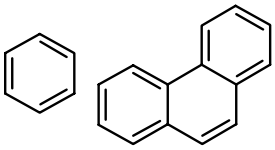
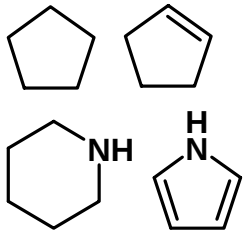
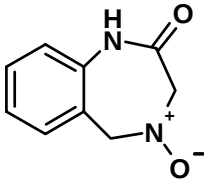
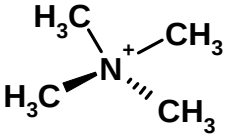
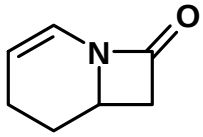
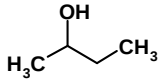
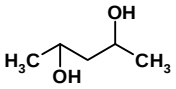
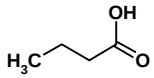
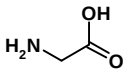
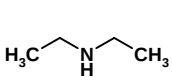
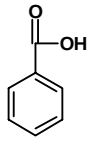
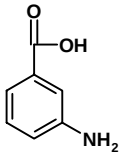
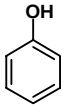
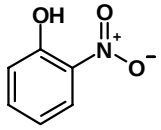
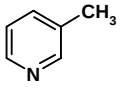
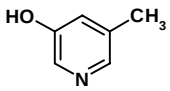
M_POL	Number of aromatic polar substituents (aromatic substituents excluding Ar-CX_2- and Ar-CX=C<, where X: is C or H.	 = 2
M_AMP	Amphoteric property; □-amino acid:1.0, amino benzoic acid: 0.5, pyridinecarboxylic acid 0.5.  = 0.5  = 0.5	 =1.0
M_ALK	Indicator variable for alkane, alkene, cycloalkane, or cycloalkene (hydrocarbons with 0 or 1 double bond) 	
M_RNG	Indicator variable for the presence of ring structures except benzene and its condensed rings (aromatic, heteroaromatic, and hydrocarbon rings).  E.g., excluded	
M_QN	Quaternary nitrogen: >N^+<: 1.0, N oxide:0.5  = 0.5	
M_NO2	Number of nitro groups	
M_NCS	Isothiocyanate (-N=C=S): 1.0, thiocyanate (-S-C#N): 0.5	
M_BLM	Indicator variable for the presence of beta-lactam.	

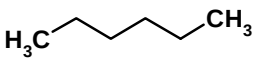
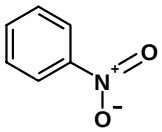
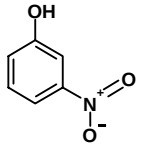
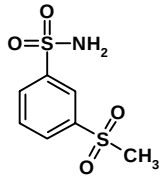
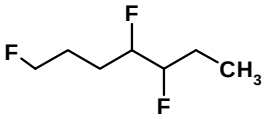
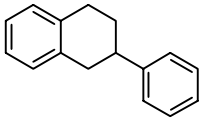
Table 5. Molecular Pattern Recognition Flags:

AlphaAA	Alpha Amino Acid Flag
PrAlphAA	Primary Alpha Amino Acid Flag
AlphaAE	Alpha Amino Ester Flag
PrAlphAE	Primary Alpha Amino Ester Flag
Steroid	Flag Indicating Steroid-like Fused Ring Subunit

Table 6. Meylan Flags for MH Sw models:

Parameter	Description	Exceptions

H_AlAlco (Aliphatic Alcohol)	Compounds with exactly one OH group attached to an aliphatic hydrocarbon 	Compounds with multiple OH, and any functional group other than OH 
H_AlAcid (Aliphatic Acid)	Compounds with one or more carboxyl groups attached to aliphatic carbons 	Amino acids (aliphatic or aromatic amines, except quaternary) and amides 
H_AlAmin (Aliphatic Amine)	Compounds with primary, secondary, or tertiary amines attached to aliphatic carbons  	Melting point greater than 25ºC
H_ArAcid (Aromatic Acid)	Compounds with at least one carboxyl group attached to an aromatic carbon 	Compounds with any amino-type substituent attached to the same ring where –COOH is attached. “Amino-type” = aliphatic nitrogen whose only attachments are carbons or other nitrogens. 
H_Phenol (Phenol)	Compounds with at least one OH attached to an aromatic carbon 	Compounds with amino-type substituent on the same ring and compounds with nitro, alkyloxy or other OH ortho to OH 
H_AlPyri (Alkylpyridine)	Compounds with at least one pyridine ring  	Only alkyl substituents allowed; carbon attached to ring must by CH_3, CH_2-, or CH< 
H_Azo (Azo)	Compounds with -N=N-	Both N’s must be attached to carbon

H_Nitrile (Nitrile)	Compounds with -C≡N	N=C-CN, C=N-CN
H_Hcarb (Hydrocarbon)	Aliphatic compounds with only C and H 	
H_Nitro (Nitro)	Aliphatic and aromatic compounds with nitro ($-NO_2$) group 	N attachment or any amino or OH substituent if nitro group is attached to aromatic ring 
H_SO2 (SO_2)	Compounds with at least one sulfonamide on aromatic ring plus an other substituent that is ketone, sulfone, or another sulfonamide on the same ring; also applies to compounds with -S(=O)-C-C(=O)-C (number of O on S is not limited) 	
H_Falkan (Fluoroalkane)	Hydrocarbon compounds with at least one fluorine 	
H_PAH (Polycyclic aromatic hydrocarbons)	Hydrocarbons with at least three rings, at least two of which must be aromatic. 	

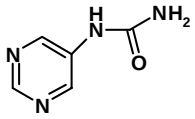
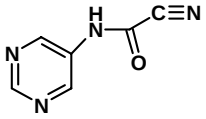
H_MultiN (Multi-N)	Compounds with at least one of the following: - four or more aromatic nitrogens - zero aromatic and two or more aliphatic nitrogens. Exactly one aliphatic N must be attached to C(=O), C(=S), or S(=O) - two or more aromatic and two or more aliphatic nitrogens. All aliphatic nitrogens must be attached to C(=O), C(=S), or S(=O) 	Compounds with at least one of the following: - sulfonamide - barbiturate - metal atom or ion  Excluded from aliphatic nitrogen count are: - nitro - nitrile - azo
H_AmAcid (Amino Acid)	Compound with at least one carboxyl and at least one amino group.	Compounds with aromatic attachment of at least one carboxyl group.

Table 7. Descriptors Derived from Electronic Properties (charge unit=absolute electron charge)

FormalQ	Formal electric charge
ABSQ	Sum of Absolute Values of PEOE Partial Atomic Charges
ABSQon	As above, but only on O and N atoms
MaxQ	Maximal PEOE Partial Atomic Charge
MinQ	Minimal PEOE Partial Atomic Charge
NPA_ABSQ	Sum of absolute values of estimated NPA partial atomic charges
NPA_AQon	As above, but only on O and N atoms
NPA_AQh	As above, but only on H atoms
NPA_AQc	As above, but only on C atoms
NPA_MaxQ	Maximal Estimated NPA Partial Atomic Charge
NPA_MinQ	Minimal Estimated NPA Partial Atomic Charge
NPA_Q1	First component of the autocorrelation vector of estimated NPA partial atomic charges
NPA_Q2	Second component of the autocorrelation vector of estimated NPA partial atomic charges
NPA_Q3	Third component of the autocorrelation vector of estimated NPA partial atomic charges
NPA_Q4	Fourth component of the autocorrelation vector of estimated NPA partial atomic charges
NPA_Q5	Fifth component of the autocorrelation vector of estimated NPA partial atomic charges
NPA_Q6	Sixth component of the autocorrelation vector of estimated NPA partial atomic charges
EEM_AFon	Sum of absolute values of sigma Fukui indices on N and O
EEM_AFc	Sum of absolute values of sigma Fukui indices on C
EEM_AFpl	Sum of absolute values of sigma Fukui indices on polar atoms
EEM_AFnp	Sum of absolute values of sigma Fukui indices on nonpolar atoms
EEM_MaxF	Maximum sigma Fukui index
EEM_XFon	Maximum sigma Fukui index on N and O

EEM_NFon	Minimum sigma Fukui index on N and O
EEM_XFh	Maximum sigma Fukui index on H
EEM_XFc	Maximum sigma Fukui index on C
EEM_NFc	Minimum sigma Fukui index on C
EEM_XFpl	Maximum sigma Fukui index on polar atoms
EEM_NFpl	Minimum sigma Fukui index on polar atoms
EEM_XFnp	Maximum sigma Fukui index on nonpolar atoms
EEM_NFnp	Minimum sigma Fukui index on nonpolar atoms
EEM_F1	First component of the autocorrelation vector of sigma Fukui indices
EEM_F2	Second component of the autocorrelation vector of sigma Fukui indices
EEM_F3	Third component of the autocorrelation vector of sigma Fukui indices
EEM_F4	Fourth component of the autocorrelation vector of sigma Fukui indices
EEM_F5	Fifth component of the autocorrelation vector of sigma Fukui indices
EEM_F6	Sixth component of the autocorrelation vector of sigma Fukui indices
Pi_ABSQ	Sum of absolute values of Hückel pi atomic charges
Pi_AQo	As above, but only on O atoms
Pi_AQn	As above, but only on N atoms
Pi_AQc	As above, but only on C atoms
Pi_MaxQ	Maximum Hückel pi atomic charge
Pi_MinQ	Minimum Hückel pi atomic charge
Pi_Q1	First component of the autocorrelation vector of Hückel pi atomic charges
Pi_Q2	Second component of the autocorrelation vector of Hückel pi atomic charges
Pi_Q3	Third component of the autocorrelation vector of Hückel pi atomic charges
Pi_Q4	Fourth component of the autocorrelation vector of Hückel pi atomic charges
Pi_Q5	Fifth component of the autocorrelation vector of Hückel pi atomic charges
Pi_Q6	Sixth component of the autocorrelation vector of Hückel pi atomic charges
Pi_AFPlc	Sum of absolute values of pi Fukui(+) indices on C
Pi_AFMic	Sum of absolute values of pi Fukui(-) indices on C
Pi_MaxFPl	Maximum pi Fukui(+) index
Pi_MaxFMi	Maximum pi Fukui(-) index
Pi_FPl1	First component of the autocorrelation vector of pi Fukui(+) indices
Pi_FPl2	Second component of the autocorrelation vector of pi Fukui(+) indices
Pi_FPl3	Third component of the autocorrelation vector of pi Fukui(+) indices
Pi_FPl4	Fourth component of the autocorrelation vector of pi Fukui(+) indices
Pi_FPl5	Fifth component of the autocorrelation vector of pi Fukui(+) indices
Pi_FPl6	Sixth component of the autocorrelation vector of pi Fukui(+)

	indices
Pi_FMi1	First component of the autocorrelation vector of pi Fukui(-) indices
Pi_FMi2	Second component of the autocorrelation vector of pi Fukui(-) indices
Pi_FMi3	Third component of the autocorrelation vector of pi Fukui(-) indices
Pi_FMi4	Fourth component of the autocorrelation vector of pi Fukui(-) indices
Pi_FMi5	Fifth component of the autocorrelation vector of pi Fukui(-) indices
Pi_FMi6	Sixth component of the autocorrelation vector of pi Fukui(-) indices
EqualChi	Equalized molecular electronegativity
EqualEta	Equalized molecular hardness
Elephity	Electrophilicity index
N_Electr	Total number of electrons in a molecule
PolarizG	Polarizability in A^3 calculated by Glen's method
PolarizM	Polarizability in A^3 calculated by Miller's method

Table 8. Hydrogen Bonding Descriptors:

IHB	Number of Intra-molecular Hydrogen Bonds
PHB	Proximity Effects of HB Donors and HB Acceptors. Similar to IHB, but counts all possible donor-acceptor pairs within the IHB range.
HBD	Number of Hydrogen Bond Donors
HBA	Number of Hydrogen Bond Acceptors
HBDo	Number of Oxygen-based Hydrogen Bond Donors
HBAo	Number of Oxygen-based Hydrogen Bond Acceptors
HBDn	Number of Nitrogen-based Hydrogen Bond Donors
HBAn	Number of Nitrogen-based Hydrogen Bond Acceptors
HBDch	Sum of Estimated NPA Partial Atomic Charges on HB Donor Hydrogens
HBAch	Sum of Estimated NPA Partial Atomic Charges on HB Acceptors
HBDoch	Sum of Estimated NPA Partial Atomic Charges on Oxygen-based HB Donor Hydrogens
HBAoch	Sum of Estimated NPA Partial Atomic Charges on Oxygen-based HB Acceptors
HBDnch	Sum of Estimated NPA Partial Atomic Charges on Nitrogen-based HB Donor Hydrogens
HBAnch	Sum of Estimated NPA Partial Atomic Charges on Nitrogen-based HB Acceptors

Table 9. Molecular Ionization Descriptors:

N_IoAcAt	Number of recognized ionizable atom types that are acidic
N_IoBaAt	Number of recognized ionizable atom types that are basic
AcidAtoms	Numeric labels and types of all detected acidic atoms (string)
BaseAtoms	Numeric labels and types of all detected basic atoms (string)
FAnion	Cumulative Contribution of Purely Anionic Species to Fraction Ionized at Specified pH (default 7.4)
FCation	Cumulative Contribution of Purely Cationic Species to Fraction Ionized at Specified pH (default 7.4)

FUnion	Cumulative Contribution of All Species with Zero Formal Charge to Fraction Ionized at Specified pH (default 7.4)
FZwitter	Portion of FUnion Contributed by Zwitterionic Species (does not depend on pH)
QAvgNeg	Absolute Value of the Population Average Across All Ionized Species of the Net Formal Negative Charge Calculated at Specified pH (default 7.4)
QAvgPos	Population Average Across All Ionized Species of the Net Formal Positive Charge Calculated at Specified pH (default 7.4)
F_NLP	Population Average Across All Ionized Species of the Number of Lone Electron Pairs on N,O,S,P, Divided by the Number of Atoms
F_HBP	Population Average Across All Ionized Species of the Number of Protons Available for Hydrogen Bonding, Divided by the Number of Atoms

Table 10. 3D Descriptors (length unit=angstrom, mass unit=dalton):

RgGrav__3D	Gravitational radius of gyration
RgGeom__3D	Geometrical radius of gyration
RadMax__3D	Distance between center of mass and the most distant atom
Propr1__3D	Simulations Plus proprietary descriptor
MIRxx___3D	Largest principal moment of inertia
MIRyy___3D	Medium principal moment of inertia
MIRzz___3D	Smallest principal moment of inertia
SM2xx___3D	Smallest principal static moment of the second order
SM2yy___3D	Medium principal static moment of the second order
SM2zz___3D	Largest principal static moment of the second order
BoxX____3D	Smallest dimension of the tightest enclosing box in A
BoxY____3D	Medium dimension of the tightest enclosing box in A
BoxZ____3D	Largest dimension of the tightest enclosing box in A
DStokes_3D	Stokes-Einstein diffusion coefficient (cm^2/s x 10^5)
Propr2__3D	Simulations Plus proprietary descriptor
Grav3___3D	Cube root of Wessel gravitational index
TotASA__3D	Total solvent accessible surface area in A^2
PolASA__3D	Polar solvent accessible surface area in A^2
NpoASA__3D	Nonpolar solvent accessible surface area in A^2
SolvE___3D	Aqueous solvation energy in kcal/mol
SolvEMt_3D	Length of the solvation energy moment vector in A*kcal/mol
PEoED___3D	Proximity effects of electron donors. Descriptor derived from Anna Seelig's work on P-glycoprotein substrate recognition patterns.
PEoEDIa_3D	Proximity effects of electron donors of type I including atoms with hydrogens. Descriptor derived from Anna Seelig's work on P-glycoprotein substrate recognition patterns.
PEoEDIb_3D	Proximity effects of electron donors of type I excluding atoms with hydrogens. Descriptor derived from Anna Seelig's work on P-glycoprotein substrate recognition patterns.
PEoEDIIa3D	Proximity effects of electron donors of type II including atoms with hydrogens. Descriptor derived from Anna Seelig's work on P-glycoprotein substrate recognition patterns.
PEoEDIIb3D	Proximity effects of electron donors of type II excluding atoms with hydrogens. Descriptor derived from Anna Seelig's work

	on P-glycoprotein substrate recognition patterns.
HBAsa___3D	Total solvent accessible surface area on HB acceptors
HBAwsa__3D	Estimated NPA charge-weighted solvent accessible surface area on HB acceptors
PosASA__3D	Positively NPA-charged solvent accessible surface area
NegASA__3D	Negatively NPA-charged solvent accessible surface area
Dipole__3D	Estimated NPA dipole moment