Appendix A

Descriptors

This Appendix is based on an overview of the QSAR descriptors in MOE (Molecular Operating Environment) by the Chemical Computing Group. Please refer to http://www.chemcomp.com/journal/descr.htm for the original source. The following list shows the sub-groups of the 2D descriptors:

- **2D Molecular Descriptors**
  - Physical Properties ($2D_{phys}$)
  - Subdivided Surface Areas ($2D_{sa}$)
  - Atom Counts and Bond Counts ($2D_{counts}$)
  - Kier & Hall Connectivity and Kappa Shape Indices ($2D_{kh}$)
  - Adjacency and Distance Matrix Descriptors ($2D_{adj}$)
  - Pharmacophore Feature Descriptors ($2D_{pharm}$)
  - Partial Charge Descriptors ($2D_{charge}$)

Table A.1: List of QSAR descriptors in the Molecular Operating Environment (MOE). The descriptions are based on the Chemical Computing Group's webpage [1]

Code	Type	Used	Description
apol	$2D_{phys}$		Sum of the atomic polarizabilities (including implicit hydrogens) with polarizabilities taken from [2].
bpol	$2D_{phys}$		Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens) with polarizabilities taken from [2].
density	$2D_{phys}$		Molecular mass density: Weight divided by vdw_vol.
FCharge	$2D_{phys}$	V	Total charge of the molecule (sum of formal charges).
mr	$2D_{phys}$		Molecular refractivity (including implicit hydrogens). This property is calculated from an 11 descriptor linear model [3] with R^2=0.997, RMSE=0.168 on 1,947 small molecules.
SMR	$2D_{phys}$		Molecular refractivity (including implicit hydrogens). This property is an atomic contribution model [4] that assumes the correct protonation state (washed structures). The model was trained on 7000 structures and results may vary from the mr descriptor.
AM1_dipole	$2D_{phys}$	R	The dipole moment calculated using the AM1 Hamiltonian [5].
AM1_E	$2D_{phys}$	R	The total energy calculated using the AM1 Hamiltonian [5].
AM1_Eele	$2D_{phys}$	R	The electronic energy calculated using the AM1 Hamiltonian [5].
AM1_HF	$2D_{phys}$	R	The heat of formation calculated using the AM1 Hamiltonian [5].
AM1_IP	$2D_{phys}$	R	The ionization potatnial calculated using the AM1 Hamiltonian [5].
AM1_HOMO	$2D_{phys}$	R	The energy of the Highest Unoccupied Molecular Orbital calculated using the AM1 Hamiltonian [5].
AM1_LUMO	$2D_{phys}$	R	The energy of the Lowest Unoccupied Molecular Orbital calculated using the AM1 Hamiltonian [5].
MNDO_dipole	$2D_{phys}$	R	The dipole moment calculated using MNDO Hamiltonian [5].
MNDO_E	$2D_{phys}$	R	The total energy calculated using the MNDO Hamiltonian [5].
MNDO_Eele	$2D_{phys}$	R	The electronic energy calculated using the MNDO Hamiltonian [5].
MNDO_HF	$2D_{phys}$	R	The heat of formation calculated using the MNDO Hamiltonian [5].
MNDO_IP	$2D_{phys}$	R	The ionization potatnial calculated using the MNDO Hamiltonian [5].
MNDO_HOMO	$2D_{phys}$	R	The energy of the Highest Unoccupied Molecular Orbital calculated using the MNDO Hamiltonian [5].
MNDO_LUMO	$2D_{phys}$	R	The energy of the Lowest Unoccupied Molecular Orbital calculated using the MNDO Hamiltonian [5].
PM3_dipole	$2D_{phys}$	U	The dipole moment calculated using PM3 Hamiltonian [5].
PM3_E	$2D_{phys}$		The total energy calculated using the PM3 Hamiltonian [5].
PM3_Eele	$2D_{phys}$		The electronic energy calculated using the PM3 Hamiltonian [5].
PM3_HF	$2D_{phys}$		The heat of formation calculated using the PM3 Hamiltonian [5].
PM3_IP	$2D_{phys}$		The ionization potatnial calculated using the PM3 Hamiltonian [5].
PM3_HOMO	$2D_{phys}$		The energy of the Highest Unoccupied Molecular Orbital calculated using the PM3 Hamiltonian [5].

PM3_LUMO	$2D_{phys}$		The energy of the Lowest Unoccupied Molecular Orbital calculated using the PM3 Hamiltonian [5].
TPSA	$2D_{phys}$		Total Polar Surface Area calculated using group contributions to approximate the polar surface area from connection table information only [6].
Weight	$2D_{phys}$		Molecular weight (including implicit hydrogens) with atomic weights taken from [2].
LogS	$2D_{phys}$	R	Log of the aqueous solubility calculated from an atom contributiontilear atom type model [7].
logP(o/w)	$2D_{phys}$		Log of the octanol/water partition coefficient (including implicit hydrogens). This property is calculated from a linear atom type model [8] with R^2=0.931, RMSE=0.393 on 1,847 molecules.
SlogP	$2D_{phys}$		Log of the octanol/water partition coefficient (including implicit hydrogens). This property is an atomic contribution model [4] that calculates logP from the given structure; i.e., the correct protonation state (washed structures). Results may vary from the logP(o/w) descriptor. The training set for SlogP was 7000 structures.
vdw_vol	$2D_{phys}$		van der Waals volume calculated using a connection table approximation.
vdw_area	$2D_{phys}$		Area of van der Waals surface calculated using a connection table approximation.
SlogP_VSA0	$2D_{sa}$		Sum of v_i such that L_i ¡= -0.4.
SlogP_VSA1	$2D_{sa}$		Sum of v_i such that L_i is in [-0.4,-0.2].
SlogP_VSA2	$2D_{sa}$	U	Sum of v_i such that L_i is in [-0.2,0].
SlogP_VSA3	$2D_{sa}$		Sum of v_i such that L_i is in [0,0.1].
SlogP_VSA4	$2D_{sa}$		Sum of v_i such that L_i is in [0.1,0.15].
SlogP_vsa5	$2D_{sa}$		Sum of v_i such that L_i is in [0.15,0.20].
SlogP_VSA6	$2D_{sa}$		Sum of v_i such that L_i is in [0.20,0.25].
SlogP_VSA7	$2D_{sa}$		Sum of v_i such that L_i is in [0.25,0.30].
SlogP_VSA8	$2D_{sa}$		Sum of v_i such that L_i is in [0.30,0.40].
SlogP_VSA9	$2D_{sa}$		Sum of v_i such that L_i ¿ 0.40.
SMR_VSA0	$2D_{sa}$		Sum of v_i such that R_i is in [0,0.11].
SMR_VSA1	$2D_{sa}$		Sum of v_i such that R_i is in [0.11,0.26].
SMR_VSA2	$2D_{sa}$		Sum of v_i such that R_i is in [0.26,0.35].
SMR_VSA3	$2D_{sa}$		Sum of v_i such that R_i is in [0.35,0.39].
SMR_VSA4	$2D_{sa}$		Sum of v_i such that R_i is in [0.39,0.44].
SMR_VSA5	$2D_{sa}$		Sum of v_i such that R_i is in [0.44,0.485].
SMR_VSA6	$2D_{sa}$		Sum of v_i such that R_i is in [0.485,0.56].
SMR_VSA7	$2D_{sa}$	U	Sum of v_i such that R_i ¿ 0.56.
nmol	$2D_{count}$	V	Number of molecules.
a_aro	$2D_{count}$		Number of aromatic atoms.
a_count	$2D_{count}$		Number of atoms (including implicit hydrogens).
a_heavy	$2D_{count}$		Number of heavy atoms($Z_i > 1$).
a_ICM	$2D_{count}$		Atom information content (mean).
a_IC	$2D_{count}$		Atom information content (total).
a_nH	$2D_{count}$		Number of hydrogen atoms (including implicit hydrogens).
a_nB	$2D_{count}$	V	Number of boron atoms.
a_nC	$2D_{count}$		Number of carbon atoms.
a_nN	$2D_{count}$		Number of nitrogen atoms.
a_nO	$2D_{count}$		Number of oxygen atoms.
a_nF	$2D_{count}$		Number of fluorine atoms.
a_nP	$2D_{count}$	V	Number of phosphorus atoms.
a_nS	$2D_{count}$		Number of sulfur atoms.
a_nCl	$2D_{count}$		Number of chlorine atoms.
a_nBr	$2D_{count}$	V	Number of bromine atoms.
a_nI	$2D_{count}$		Number of iodine atoms.
b_1rotN	$2D_{count}$	U	Number of rotatable single bonds.
b_1rotR	$2D_{count}$		Fraction of rotatable single bonds.
b_ar	$2D_{count}$		Number of aromatic bonds.
b_count	$2D_{count}$		Number of bonds (including implicit hydrogens).

b_double	$2D_{count}$	U	Number of double bonds. Aromatic bonds are not considered to be double bonds.
b_heavy	$2D_{count}$		Number of bonds between heavy atoms.
b_rotN	$2D_{count}$		Number of rotatable bonds.
b_rotR	$2D_{count}$		Fraction of rotatable bonds.
b_single	$2D_{count}$		Number of single bonds (including implicit hydrogens). Aromatic bonds are not considered to be single bonds.
b_triple	$2D_{count}$		Number of triple bonds.
VAdjMa	$2D_{count}$		Vertex adjacency information (magnitude): $1 + log_2 m$ where m is the number of heavy-heavy bonds. If m is zero, then zero is returned.
VAdjEq	$2D_{count}$		Vertex adjacency information (equality): $-(1-f)log_2(1-f) - flog_2 f$ where $f = (n^2 - m)/n^2$, n is the number of heavy atoms and m is the number of heavy-heavy bonds. If f is not in the open interval (0,1), then 0 is returned.
lip_acc	$2D_{counts}$		Number of O and N atoms.
lip_don	$2D_{counts}$		Number of OH and NH atoms.
lip_druglike	$2D_{counts}$	R	1 if $lip\_violation < 2$ otherwise 0.
lip_violation	$2D_{counts}$	R	Number of violations of Lipinski's Rule of Five [9].
opr_brigid	$2D_{counts}$		Number of rigid bonds [10].
opr_nring	$2D_{counts}$		Number of ring bonds [10].
opr_nrot	$2D_{counts}$		Number of rotatable bonds [10].
opr_leadlike	$2D_{counts}$	R	1 if $opr\_violation < 2$ otherwise 0.
opr_violation	$2D_{counts}$	R	Number of violations of Oprea's lead-like test [10].
chi0	$2D_{kh}$		Atomic connectivity index (order 0) [11, 12].
chi0_C	$2D_{kh}$		Carbon connectivity index (order 0).
chi1	$2D_{kh}$		Atomic connectivity index (order 1) [11, 12].
chi1_C	$2D_{kh}$		Carbon connectivity index (order 1).
chi0v	$2D_{kh}$		Atomic valence connectivity index (order 0) [11, 12].
chi0v_C	$2D_{kh}$		Carbon valence connectivity index (order 0).
chi1v	$2D_{kh}$		Atomic valence connectivity index (order 1) [11, 12].
chi1v_C	$2D_{kh}$		Carbon valence connectivity index (order 1).
Kier1	$2D_{kh}$		First kappa shape index [11].
Kier2	$2D_{kh}$		Second kappa shape index [11].
Kier3	$2D_{kh}$		Third kappa shape index [11].
KierA1	$2D_{kh}$		First alpha modified shape index [11].
KierA2	$2D_{kh}$		Second alpha modified shape index [11].
KierA3	$2D_{kh}$		Third alpha modified shape index [11].
KierFlex	$2D_{kh}$		Kier molecular flexibility index [11].
zagreb	$2D_{kh}$		Zagreb index.
balabanJ	$2D_{adj}$		Balaban's connectivity topological index [13].
diameter	$2D_{adj}$		Largest value in the distance matrix [14].
petitjean	$2D_{adj}$		Value of (diameter-radius) / diameter as defined in [14].
radius	$2D_{adj}$		Radius is defined as the smallest of the r_i [14].
BCUT_PEOE_0	$2D_{adj}$		The BCUT descriptors are calculated from the eigenvalues of a modified adjancy matrix [15]. Smallest eigenvalue.
BCUT_PEOE_1	$2D_{adj}$		The BCUT descriptors are calculated from the eigenvalues of a modified adjancy matrix [15]. 1/3-ile eigenvalue.
BCUT_PEOE_2	$2D_{adj}$		The BCUT descriptors are calculated from the eigenvalues of a modified adjancy matrix [15]. 2/3-ile eigenvalue.
BCUT_PEOE_3	$2D_{adj}$		The BCUT descriptors are calculated from the eigenvalues of a modified adjancy matrix [15]. Largest eigenvalue.
BCUT_SLOGP_0	$2D_{adj}$		The BCUT descriptors using LogP contribution instead of partial charge. Smallest eigenvalue.
BCUT_SLOGP_1	$2D_{adj}$		The BCUT descriptors using LogP contribution instead of partial charge. 1/3-ile eigenvalue.
BCUT_SLOGP_2	$2D_{adj}$		The BCUT descriptors using LogP contribution instead of partial charge. 2/3-ile eigenvalue.
BCUT_SLOGP_3	$2D_{adj}$		The BCUT descriptors using LogP contribution instead of partial charge. Largest eigenvalue.
BCUT_SMR_0	$2D_{adj}$		The BCUT descriptors using atomic contribution to molar refractivity instead of partial charge. Smallest eigenvalue.

BCUT_SMR_1	$2D_{adj}$		The BCUT descriptors using atomic contribution to molar refractivity instead of partial charge. 1/3-ile eigenvalue.
BCUT_SMR_2	$2D_{adj}$		The BCUT descriptors using atomic contribution to molar refractivity instead of partial charge. 2/3-ile eigenvalue.
BCUT_SMR_3	$2D_{adj}$		The BCUT descriptors using atomic contribution to molar refractivity instead of partial charge. Largest eigenvalue.
GCUT_PEOE_0	$2D_{adj}$		The GCUT descriptors are calculated from the eigenvalues of a modified graph distance adjancy matrix. Smallest eigenvalue.
GCUT_PEOE_1	$2D_{adj}$		The GCUT descriptors are calculated from the eigenvalues of a modified graph distance adjancy matrix. 1/3-ile eigenvalue.
GCUT_PEOE_2	$2D_{adj}$	U	The GCUT descriptors are calculated from the eigenvalues of a modified graph distance adjancy matrix. 2/3-ile eigenvalue.
GCUT_PEOE_3	$2D_{adj}$		The GCUT descriptors are calculated from the eigenvalues of a modified graph distance adjancy matrix. Largest eigenvalue.
GCUT_SLOGP_0	$2D_{adj}$		The GCUT descriptors using LogP contribution instead of partial charge. Smallest eigenvalue.
GCUT_SLOGP_1	$2D_{adj}$		The GCUT descriptors using LogP contribution instead of partial charge. 1/3-ile eigenvalue.
GCUT_SLOGP_2	$2D_{adj}$		The GCUT descriptors using LogP contribution instead of partial charge. 2/3-ile eigenvalue.
GCUT_SLOGP_3	$2D_{adj}$		The GCUT descriptors using LogP contribution instead of partial charge. Largest eigenvalue.
GCUT_SMR_0	$2D_{adj}$		The GCUT descriptors using atomic contribution to molar refractivity instead of partial charge. Smallest eigenvalue.
GCUT_SMR_1	$2D_{adj}$		The GCUT descriptors using atomic contribution to molar refractivity instead of partial charge. 1/3-ile eigenvalue.
GCUT_SMR_2	$2D_{adj}$		The GCUT descriptors using atomic contribution to molar refractivity instead of partial charge. 2/3-ile eigenvalue.
GCUT_SMR_3	$2D_{adj}$		The GCUT descriptors using atomic contribution to molar refractivity instead of partial charge. Largest eigenvalue.
VDistEq	$2D_{adj}$		VdistEq is defined as the sum of $log_2 m - log_2 p_i/m$ where p_i is the number of distance matrix entries equal to i.
VDistMa	$2D_{adj}$		VDistMa is defined as the sum of $log_2 m - D_{ij} log_2 D_{ij}/m$ over all i and j.
weinerPath	$2D_{adj}$		Wiener path number [16, 17].
weinerPol	$2D_{adj}$		Wiener polarity number [16].
a_acc	$2D_{pharm}$		Number of hydrogen bond acceptor atoms (not counting acidic atoms but counting atoms that are both hydrogen bond donors and acceptors such as -OH).
a_acid	$2D_{pharm}$	V	Number of acidic atoms.
a_base	$2D_{pharm}$	V	Number of basic atoms.
a_don	$2D_{pharm}$		Number of hydrogen bond donor atoms (not counting basic atoms but counting atoms that are both hydrogen bond donors and acceptors such as -OH).
a_hyd	$2D_{pharm}$		Number of hydrophobic atoms.
vsa_acc	$2D_{pharm}$		Approximation to the sum of VDW surface areas of pure hydrogen bond acceptors (not counting acidic atoms and atoms that are both hydrogen bond donors and acceptors such as -OH).
vsa_acid	$2D_{pharm}$	V	Approximation to the sum of VDW surface areas of acidic atoms.
vsa_base	$2D_{pharm}$	V	Approximation to the sum of VDW surface areas of basic atoms.
vsa_don	$2D_{pharm}$		Approximation to the sum of VDW surface areas of pure hydrogen bond donors (not counting basic atoms and atoms that are both hydrogen bond donors and acceptors such as -OH).

vsa_hyd	$2D_{pharm}$		Approximation to the sum of VDW surface areas of hydrophobic atoms.
vsa_other	$2D_{pharm}$		Approximation to the sum of VDW surface areas of atoms typed as "other".
vsa_pol	$2D_{pharm}$		Approximation to the sum of VDW surface areas of polar (both hydrogen bond donors and acceptors) atoms (such as -OH).
PC+	$2D_{charge}$		Total positive partial charge (Suffix: Q for external charges, PEOE for calculated charges).
PC-	$2D_{charge}$	U	Total negative partial charge (Suffix: Q for external charges, PEOE for calculated charges).
RPC+	$2D_{charge}$		Relative positive partial charge (Suffix: Q for external charges, PEOE for calculated charges).
PRC-	$2D_{charge}$		Relative negative partial charge (Suffix: Q for external charges, PEOE for calculated charges).
VSA_POS	$2D_{charge}$	U	Total positive van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_NEG	$2D_{charge}$		Total negative van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_PPOS	$2D_{charge}$		Total positive polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_PNEG	$2D_{charge}$		Total negative polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_HYD	$2D_{charge}$		Total hydrophobic van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_POL	$2D_{charge}$		Total polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FPOS	$2D_{charge}$		Fractional positive van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FNEG	$2D_{charge}$		Fractional negative van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FPPOS	$2D_{charge}$		Fractional positive polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FPNEG	$2D_{charge}$		Fractional negative polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FHYD	$2D_{charge}$		Fractional hydrophobic van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
VSA_FPOL	$2D_{charge}$		Fractional polar van der Waals surface area (Suffix: Q for external charges, PEOE for calculated charges).
PEOE_VSA+6	$2D_{charge}$		Sum of v_i where q_i is greater than 0.3.
PEOE_VSA+5	$2D_{charge}$		Sum of v_i where q_i is in the range [0.25,0.30].
PEOE_VSA+4	$2D_{charge}$		Sum of v_i where q_i is in the range [0.20,0.25].
PEOE_VSA+3	$2D_{charge}$		Sum of v_i where q_i is in the range [0.15,0.20].
PEOE_VSA+2	$2D_{charge}$		Sum of v_i where q_i is in the range [0.10,0.15].
PEOE_VSA+1	$2D_{charge}$		Sum of v_i where q_i is in the range [0.05,0.10].
PEOE_VSA+0	$2D_{charge}$		Sum of v_i where q_i is in the range [0.00,0.05].
PEOE_VSA-0	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.05,0.00].
PEOE_VSA-1	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.10,-0.05].
PEOE_VSA-2	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.15,-0.10].
PEOE_VSA-3	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.20,-0.15].
PEOE_VSA-4	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.25,-0.20].
PEOE_VSA-5	$2D_{charge}$		Sum of v_i where q_i is in the range [-0.30,-0.25].
PEOE_VSA-6	$2D_{charge}$		Sum of v_i where q_i is less than -0.30.
E	$3D_{Epot}$		Value of the potential energy.
E_ang	$3D_{Epot}$		Angle bend potential energy.
E_ele	$3D_{Epot}$		Electrostatic component of the potential energy.
E_nb	$3D_{Epot}$		Value of the potential energy with all non-bonded terms disabled.
E_oop	$3D_{Epot}$		Out-of-plane potential energy.
E_sol	$3D_{Epot}$	U	Solvation energy.
E_stb	$3D_{Epot}$		Bond stretch-bend cross-term potential energy.
E_str	$3D_{Epot}$		Bond stretch potential energy.

E_strain	$3D_{Epot}$		Local strain energy: the current energy minus the value of the energy at a near local minimum.
E_tor	$3D_{Epot}$		Torsion potential energy.
E_vdw	$3D_{Epot}$		van der Waals component of the potential energy.
E_rele	$3D_{Epot}$	V	Electrostatic interaction energy (x3d).
E_rnb	$3D_{Epot}$	V	Non-bonded interaction energy (x3d).
E_rsol	$3D_{Epot}$	V	Solvation free energy difference (x3d).
E_rvdw	$3D_{Epot}$	V	van der Waals interaction energy (x3d).
ASA	$3D_{shape}$		Water accessible surface area calculated using a radius of 1.4 A for the water molecule.
dens	$3D_{shape}$		Mass density: molecular weight divided by van der Waals volume.
glob	$3D_{shape}$		Globularity, or inverse condition number of the covariance matrix of atomic coordinates.
pmi	$3D_{shape}$		Principal moment of inertia.
pmiX	$3D_{shape}$		x component of the principal moment of inertia (x3d).
pmiY	$3D_{shape}$		y component of the principal moment of inertia (x3d).
pmiZ	$3D_{shape}$		z component of the principal moment of inertia (x3d).
rgyr	$3D_{shape}$		Radius of gyration.
std_dim1	$3D_{shape}$		Standard dimension 1: the square root of the largest eigenvalue of the covariance matrix of the atomic coordinates.
std_dim2	$3D_{shape}$		Standard dimension 2: the square root of the second largest eigenvalue of the covariance matrix of the atomic coordinates.
std_dim3	$3D_{shape}$		Standard dimension 3: the square root of the third largest eigenvalue of the covariance matrix of the atomic coordinates.
vol	$3D_{shape}$		van der Waals volume calculated using a grid approximation (spacing 0.75 A).
VSA	$3D_{shape}$		van der Waals surface area.
ASA+	$3D_{conf}$		Water accessible surface area of all atoms with positive partial charge.
ASA-	$3D_{conf}$		Water accessible surface area of all atoms with negative partial charge.
ASA_H	$3D_{conf}$		Water accessible surface area of all hydrophobic atoms.
ASA_P	$3D_{conf}$		Water accessible surface area of all polar atoms.
DASA	$3D_{conf}$		Absolute value of the difference between ASA+ and ASA-.
CASA+	$3D_{conf}$		Positive charge weighted surface area [18].
CASA-	$3D_{conf}$		Negative charge weighted surface area [18].
DCASA	$3D_{conf}$		Absolute value of the difference between CASA+ and CASA- [18].
dipole	$3D_{conf}$		Dipole moment calculated from the partial charges of the molecule.
dipoleX	$3D_{conf}$		The x component of the dipole moment (x3D).
dipoleY	$3D_{conf}$		The y component of the dipole moment (x3D).
dipoleZ	$3D_{conf}$		The z component of the dipole moment (x3D).
FASA+	$3D_{conf}$		Fractional ASA+ calculated as ASA+ / ASA.
FASA-	$3D_{conf}$		Fractional ASA- calculated as ASA- / ASA.
FCASA+	$3D_{conf}$		Fractional CASA+ calculated as CASA+ / ASA.
FCASA-	$3D_{conf}$		Fractional CASA- calculated as CASA- / ASA.
FASA_H	$3D_{conf}$		Fractional ASA_H calculated as ASA_H / ASA.
FASA_P	$3D_{conf}$		Fractional ASA_P calculated as ASA_P / ASA.

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