3.4 Descriptor summary table

	GENERATOR	No.	2D/3D	Abbrev.	DESCRIPTOR NAME
1	AVERAGE	1	2D	AVERAGE	Average Energy Resulting from All Group Energies
2	CHARGE	SIGMA/PI CHARGE ELECTRONIC DESCRIPTORS			
		1	2D	QSUM	Sum of absolute value of atomic charges
		2	2D	QPOS	Charge of the most positive atom
		3	2D	QNEG	Charge of the most negative atom
		4	3D	DPOL	Electric dipole moment
3	CPSA	CHARGED PARTIAL-SURFACE-AREA DESCRIPTOR			
		1	3D	PPSA1	Partial positive surface area
		2	3D	PPSA2	Total charge weighted PPSA
		3	3D	PPSA3	Atomic charge weighted PPSA
		4	3D	PNSA1	Partial negative surface area
		5	3D	PNSA2	Total charge weighted PNSA
		6	3D	PNSA3	Atomic charge weighted PNSA
		7	3D	DPSA1	Difference of PPSA-I and PNSA-I
		8	3D	DPSA2	Difference of FPSA-2 and PNSA-2
		9	3D	DPSA3	Difference of PPSA-3 and PNSA-3
		10	3D	FPSA1	Fractional positive charged partial SA
		11	3D	FPSA2	Fractional positive charged partial SA
		12	3D	FPSA3	Fractional positive charged partial SA
		13	3D	FNSA1	Fractional negative charged partial SA
		14	3D	FNSA2	Fractional negative charged partial SA
		15	3D	FNSA3	Fractional negative charged partial SA
		16	3D	WPSA1	Weighted positive charged partial SA
		17	3D	WPSA2	Weighted positive charged partial SA
		18	3D	WPSA3	Weighted positive charged partial SA
		19	3D	WNSA1	Weighted negative charged partial SA
		20	3D	WNSA2	Weighted negative charged partial SA
		21	3D	WNSA3	Weighted negative charged partial SA
		22	2D	RPCG	Relative positive charge
		23	2D	RNCG	Relative negative charge
		24	3D	RPCS	Relative positive charged SA
		25	3D	RNCS	Relative negative charged SA
4	CPSA_AM1	CHARGED PARTIAL-SURFACE-AREA DESCRIPTOR(MOPAC AM1)			
		1	3D	PPSA1_AM1	Partial positive surface area (AM1)

		2	3D	PPSA2_AM1	Total charge weighted PPSA (AM1)
		3	3D	PPSA3_AM1	Atomic charge weighted PPSA (AM1)
		4	3D	PNSA_AM1	Partial negative surface area (AM1)
		5	3D	PNSA2_AM1	Total charge weighted PNSA (AM1)
		6	3D	PNSA3_AM1	Atomic charge weighted PNSA (AM1)
		7	3D	DPSA1_AM1	Difference of PPSA-I and PNSA-I (AM1)
		8	3D	DPSA2_AM1	Difference of FPSA-2 and PNSA-2 (AM1)
		9	3D	DPSA3_AM1	Difference of PPSA-3 and PNSA-3 (AM1)
		10	3D	FPSA1_AM1	Fractional positive charged partial SA (AM1)
		11	3D	FPSA2_AM1	Fractional positive charged partial SA (AM1)
		12	3D	FPSA3_AM1	Fractional positive charged partial SA (AM1)
		13	3D	FNSA1_AM1	Fractional negative charged partial SA (AM1)
		14	3D	FNSA2_AM1	Fractional negative charged partial SA (AM1)
		15	3D	FNSA3_AM1	Fractional negative charged partial SA (AM1)
		16	3D	WPSA1_AM1	Weighted positive charged partial SA (AM1)
		17	3D	WPSA2_AM1	Weighted positive charged partial SA (AM1)
		18	3D	WPSA3_AM1	Weighted positive charged partial SA (AM1)
		19	3D	WNSA1_AM1	Weighted negative charged partial SA (AM1)
		20	3D	WNSA2_AM1	Weighted negative charged partial SA (AM1)
		21	3D	WNSA3_AM1	Weighted negative charged partial SA (AM1)
		22	2D	RPCG_AM1	Relative positive charge (AM1)
		23	2D	RNCG_AM1	Relative negative charge (AM1)
		24	3D	RPCS_AM1	Relative positive charged SA(AM1)
		25	3D	RNCS_AM1	Relative negative charged SA (AM1)
5	CTYPE	“C"arbon "TYPE”			
		1	2D	1SP1	Primary sp1 carbon count
		2	2D	2SP1	Secondary sp1 carbon count
		3	2D	1SP2	Primary sp2 carbon count
		4	2D	2SP2	Secondary sp2 carbon count
		5	2D	3SP2	Tertiary sp2 carbon count
		6	2D	1SP3	Primary sp3 carbon count
		7	2D	2SP3	Secondary sp3 carbon count
		8	2D	3SP3	Tertiary sp3 carbon count
		9	2D	4SP3	Quaternary sp3 carbon count
6	DATOM	Atom-specific CPSA descriptors			
		1	2D	CARB-1	Average charge on carbonyl carbons
		2	2D	CARB-2	Average charge on cyano carbons
		3	3D	NITR-1	N: Partial atomic surface area

		4	3D	NITR-2	N: Total charge weighted surface area
		5	3D	NITR-3	N: Atomic charge weighted atomic surface area
		6	3D	NITR-4	N: Partial atomic surface area / total molecular surface area
		7	3D	NITR-5	N: Atomic charge weighted atomic surface area / total molecular surface area
		8	3D	OXYG-1	O: Partial atomic surface area
		9	3D	OXYG-2	O: Total charge weighted surface area
		10	3D	OXYG-3	O: Atomic charge weighted atomic surface area
		11	3D	OXYG-4	O: Partial atomic surface area / total molecular surface area
		12	3D	OXYG-5	O: Atomic charge weighted atomic surface area / total molecular surface area
		13	3D	SULF-1	S: Partial atomic surface area
		14	3D	SULF-2	S: Total charge weighted surface area
		15	3D	SULF-3	S: Atomic charge weighted atomic surface area
		16	3D	SULF-4	S: Partial atomic surface area / total molecular surface area
		17	3D	SULF-5	S: Atomic charge weighted atomic surface area / total molecular surface area
		18	3D	HALO-1	X: Partial atomic surface area
		19	3D	HALO-2	X: Total charge weighted surface area
		20	3D	HALO-3	X: Atomic charge weighted atomic surface area
		21	3D	HALO-4	X: Partial atomic surface area / total molecular surface area
		22	3D	HALO-5	X: Atomic charge weighted atomic surface area / total molecular surface area
7	DEDGE	Molecular Distance Edge Descriptor			
		1	2D	MDE 11	Molecular distance edge between all primary C
		2	2D	MDE 12	Molecular distance edge between all primary sec C
		3	2D	MDE 13	Molecular distance edge between all primary tetr C
		4	2D	MDE 14	Molecular distance edge between all primary quat C
		5	2D	MDE 22	Molecular distance edge between all sec sec C
		6	2D	MDE 23	Molecular distance edge between all sec tert C
		7	2D	MDE 24	Molecular distance edge between all sec quat C
		8	2D	MDE 33	Molecular distance edge between all tert tert C
		9	2D	MDE 34	Molecular distance edge between all tert quat C
		10	2D	MDE 44	Molecular distance edge between all quat quat C
8	DESTAT	ELECTRO-TOPOLOGICAL STATUS INDEX DESCRIPTOR			
		1	2D	EMIN 1	Minimum E-state value

		2	2D	EMAX 1	Maximum E-state value
		3	2D	EAVE 1	Average E-state value over all heavy atoms
		4	2D	EAVE 2	Average E-state value over all hetero-atoms
		5	2D	ESUM 1	Sum of E-state values over all heavy atoms
		6	2D	ESUM 2	Sum of e-state values over all hetero-atoms
		7	3D	EDIF 1	Intermolecular distance between Emin and Emax
		8	2D	ELOW 1	Difference between Min and Max E-state values
9	DFLEX	a measure of the conformational flexibility			
		1	2D	FLEX 1	Molecular mass of rigid atoms
		2	2D	FLEX 2	Molecular mass of rotatable atoms
		3	2D	FLEX 3	Fractional mass of rigid atoms
		4	2D	FLEX 4	Fractional mass of rotatable atoms
		5	3D	FLEX 5	Distance weighted flexibility
10	DGRAV	GRAVITATIONAL INDEX DESCRIPTOR			
		1	3D	GRAV 1	Gravitation index heavy atoms (HA)
		2	3D	GRAV 2	Square root gravitation index (HA)
		3	3D	GRAV 3	Cube root gravitation index (HA)
		4	3D	GRAVH 1	Gravitation index hydrogens included (HI)
		5	3D	GRAVH 2	Square root gravitation index (HI)
		6	3D	GRAVH 3	Cube root gravitation index (HI)
11	DKAPPA	CALCULATION OF KAPPA INDEXES			
		1	2D	KAPPA1	Kappa 1 index
		2	2D	KAPPA2	Kappa 2 index
		3	2D	KAPPA3	Kappa 3 index
		4	2D	KAPPA1-A	Kappa 1 index (heteroatom corrected)
		5	2D	KAPPA2-A	Kappa 2 index (heteroatom corrected)
		6	2D	KAPPA3-A	Kappa 3 index (heteroatom corrected)
12	DMALP	PATH COUNT AND LENGTH DESCRIPTORS			
		1	2D	ALLP1	Total number of paths in structure
		2	2D	ALLP2	ALLP 1/number of atoms in structure
		3	2D	ALLP3	Weighted paths in structure
		4	2D	ALLP4	ALLP 3/number of atoms in structure
		5	2D	ALLP5	the Wiener number (W)
13	DMCHI	MOLECULAR CONNECTIVITY CALCULATIONS			
		1	2D	N2P	2nd order path MC Number
		2	2D	N3P	3rd order path MC Number
		3	2D	N4P	4th order path MC Number
		4	2D	N5P	5th order path MC Number

		5	2D	N6P	6th order path MC Number
		6	2D	N2C	2nd order cluster MC Number
		7	2D	N3C	3rd order cluster MC Number
		8	2D	N4C	4th order cluster MC Number
		9	2D	N5C	5th order cluster MC Number
		10	2D	N6C	6th order cluster MC Number
		11	2D	N2PC	2nd order path-cluster MC Number
		12	2D	N3PC	3rd order path-cluster MC Number
		13	2D	N4PC	4th order path-cluster MC Number
		14	2D	N5PC	5th order path-cluster MC Number
		15	2D	N6PC	6th order path-cluster MC Number
		16	2D	N3CH	3rd order chain MC Number
		17	2D	N4CH	4th order chain MC Number
		18	2D	N5CH	5th order chain MC Number
		19	2D	N6CH	6th order chain MC Number
		20	2D	N7CH	7th order chain MC Number
		21	2D	S0	Zero-order MC (Molecular-Connectivity) Simple
		22	2D	S1	1st order MC (Molecular-Connectivity) Simple
		23	2D	S2	2nd order path MC Simple
		24	2D	S3P	3rd order path MC Simple
		25	2D	S4P	4th order path MC Simple
		26	2D	S5P	5th order path MC Simple
		27	2D	S6P	6th order path MC Simple
		28	2D	S3C	3rd order cluster MC Simple
		29	2D	S4C	4th order cluster MC Simple
		30	2D	S5C	5th order cluster MC Simple
		31	2D	S6C	6th order cluster MC Simple
		32	2D	S4PC	4th order path-cluster MC Simple
		33	2D	S5PC	5th order path-cluster MC Simple
		34	2D	S6PC	6th order path-cluster MC Simple
		35	2D	S3CH	3rd order chain MC Simple
		36	2D	S4CH	4th order chain MC Simple
		37	2D	S5CH	5th order chain MC Simple
		38	2D	S6CH	6th order chain MC Simple
		39	2D	S7CH	7th order chain MC Simple
		40	2D	V0	Zero-order MC (Molecular-Connectivity) Valence
		41	2D	V1	1st order MC (Molecular-Connectivity) Valence
		42	2D	V2	2nd order path MC Valence

		43	2D	V3P	3rd order path MC Valence
		44	2D	V4P	4th order path MC Valence
		45	2D	V5P	5th order path MC Valence
		46	2D	V6P	6th order path MC Valence
		47	2D	V3C	3rd order cluster MC Valence
		48	2D	V4C	4th order cluster MC Valence
		49	2D	V5C	5th order cluster MC Valence
		50	2D	V6C	6th order cluster MC Valence
		51	2D	V4PC	4th order path-cluster MC Valence
		52	2D	V5PC	5th order path-cluster MC Valence
		53	2D	V6PC	6th order path-cluster MC Valence
		54	2D	V3CH	3rd order chain MC Valence
		55	2D	V4CH	4th order chain MC Valence
		56	2D	V5CH	5th order chain MC Valence
		57	2D	V6CH	6th order chain MC Valence
		58	2D	V7CH	7th order chain MC Valence
14	DMCON	MOLECULAR CONNECTIVITY DESCRIPTORS			
		1	2D	MOLC1	Path-1 molecular connectivity
		2	2D	MOLC2	Path-1 ring-corrected molecular connectivity
		3	2D	MOLC3	Path-1 valence molecular connectivity
		4	2D	MOLC4	Path-2 molecular connectivity
		5	2D	MOLC5	Path-3 molecular connectivity
		6	2D	MOLC6	Path-4 molecular connectivity
		7	2D	MOLC7	Cluster-3 molecular connectivity
		8	2D	MOLC8	Path-cluster-4 molecular connectivity
		9	2D	MOLC9	Balabans topological index J
15	DMELEC	SUBSTRUCTURE DEL-RE ELECTRONIC DESCRIPTORS			
		1	2D	SCAV	Average sigma charge of atoms in the substructure
		2	2D	SCMP	Most positive sigma charge of atoms in the substructure
		3	2D	SCMN	Most negative sigma charge of atoms in the substructure
		4	2D	SCSA	Sigma charge at the specified atom in the substructure
16	DMFRAG	FRAGMENT DESCRIPTORS GENERATION ROUTINE			
		1	2D	NATM	Number of nonhydrogen atoms
		2	2D	NC	Number of Carbon atoms
		3	2D	NO	Number of Oxygen atoms
		4	2D	NN	Number of Nitrogen atoms
		5	2D	NS	Number of Sulfur atoms

		6	2D	NF	Number of Fluorine atoms
		7	2D	NCL	Number of Chlorine atoms
		8	2D	NBR	Number of Bromine atoms
		9	2D	NI	Number of Iodine atoms
		10	2D	NP	Number of Phosphorus atoms
		11	2D	NBND	Number of bonds
		12	2D	NSB	Number of single bonds
		13	2D	NDB	Number of double bonds
		14	2D	NTB	Number of triple bonds
		15	2D	NAB	Number of aromatic bonds
		16	2D	MW	Molecular weight
		17	2D	NBR	Number of basis rings
		18	2D	NRA	Number of ring atoms
		19	2D	NLP	Number of lone pairs of electrons
17	DMGEO	GEOMETRIC MOMENTS OF MOLECULES			
		1	3D	GEOM1	Mass weighted Length
		2	3D	GEOM2	Mass weighted Width
		3	3D	GEOM3	Mass weighted Thickness
		4	3D	GEOM4	Mass weighted Length/Width
		5	3D	GEOM5	Mass weighted Length/Thickness
		6	3D	GEOM6	Mass weighted Width/Thickness
18	DMOMI	MOMENTS OF INERTIA OF MOLECULES			
		1	3D	MOMI1	First moment of inertia
		2	3D	MOMI2	Second moment of inertia
		3	3D	MOMI3	Third moment of inertia
		4	3D	MOMI4	First/second moment of inertia
		5	3D	MOMI5	First/third moment of inertia
		6	3D	MOMI6	Second/third moment of inertia
		7	3D	MOMI7	Radius of gyration
		8	3D	MOMH1	First moment of inertia with H
		9	3D	MOMH2	Second moment of inertia with H
		10	3D	MOMH3	Third moment of inertia with H
		11	3D	MOMH4	First/second moment of inertia with H
		12	3D	MOMH5	First/third moment of inertia with H
		13	3D	MOMH6	Second/third moment of inertia with H
		14	3D	MOMH7	Radius of gyration with H
19	DMPATH	SUBSTRUCTURE ALL-PATH DESCRIPTORS			
		1	2D	PATH_SSS	Count of substructure (DMPATH)

		2	2D	PATH	All-path calc for substructure
20	DMREF	Molar refractivity environment of the substructure			
		1	2D	ENMR	Molar refractivity environment of the substructure
21	DMSSS	SUBSTRUCTURE COUNT AND ENVIRONMENT			
		1	2D	SSS	Count of substructure (DMSSS)
		2	2D	ENVR	Environment molecular connectivity of substructure
22	DMVOL	COMPUTE MOLECULAR VOLUME			
		1	2D	MOLV	Molecular Volume
23	DMWP	Weighted paths descriptor routine			
		1	2D	WTPT1	Molecular ID for the molecule
		2	2D	WTPT2	WTPT 1/number of atoms in the structure
		3	2D	WTPT3	Sum of atom IDs for all heteroatoms
		4	2D	WTPT4	Sum of atom IDs for oxygen atoms
		5	2D	WTPT5	Sum of atom IDs for nitrogen atoms
24	DPEND	Super-pendentic Index Descriptor			
		1	2D	PND 1	Superpendentivity index
		2	2D	PND 2	Superpendentivity index Carbon only
		3	2D	PND 3	Superpendentivity index Nitrogen only
		4	2D	PND 4	Superpendentivity index Sulfur only
		5	2D	PND 5	Superpendentivity index Oxygen only
		6	2D	PND 6	Superpendentivity index Halogen only
25	DSC	SIGMA CHARGE DESCRIPTORS			
		1	2D	TSCH	Total absolute sigma charge of atoms in structure
		2	3D	CSEP	Dist between most (+) and most (-) charge in structure
		3	2D	EDEN	Total electron density of atoms in structure
26	DSYM	SYMMETRY DESCRIPTOR			
		1	2D	SYMM1	Topological symmetry
		2	3D	SYMM2	Geometrical symmetry
		3	3D	SYMM3	Combined symmetry
27	ECCEN	Eccentric Connectivity			
		1	2D	ECCN	Eccentric connectivity index for molecule
28	FQLOGP				
		1	2D	FQLOGP	Calculate of LogP (Meylan, Howard)
	FQLOGS				
		1	2D	FQLOGS	Calculate of LogS
29	GEOWIND	3D WIENER INDEX CALCULATIONS			
		1	3D	WIEN3D	3-D Wiener Index Calculations

30	HBMIX	HYDROGEN BOND SPECIFIC DESCRIPTORS FOR MIXED COMPOUNDS			
		1	3D	MPSADH-1	Sum of surface area on donated hydrogens
		2	3D	MPSADH-2	Sum of surface area on donated hydrogens / number of donated hydrogens
		3	3D	MPSADH-3	Sum of surface area on donated hydrogens / total molecular surface area
		4	2D	MPCHDH-1	Sum of charges on all donated hydrogens
		5	2D	MPCHDH-2	Sum of charges on all donated hydrogens / number of donated hydrogens
		6	3D	MPCHDH-3	Sum of charges on all donated hydrogens / total molecular surface area
		7	3D	MPSCDH-1	Sum of (surface area * charges) on donated hydrogens
		8	3D	MPSCDH-2	Sum of (surface area * charges) on donated hydrogens / number of donated hydrogens
		9	3D	MPSCDH-3	Sum of (surface area * charges) on donated hydrogens / total molecular surface area
		10	2D	MPSAAA-1	Sum of surface area on acceptor atoms
		11	2D	MPSAAA-2	Sum of surface area on acceptor atoms / number of acceptor atoms
		12	3D	MPSAAA-3	Sum of surface area on acceptor atoms / total molecular surface area
		13	3D	MPCHAA-1	Sum of charges on acceptor atoms
		14	3D	MPCHAA-2	Sum of charges on acceptor atoms / number of acceptor atoms
		15	3D	MPCHAA-3	Sum of charges on acceptor atoms / total molecular surface area
		16	3D	MPSCAA-1	Sum of (surface area * charges) on acceptor atoms
		17	3D	MPSCAA-2	Sum of (surface area * charges) on acceptor atoms / number of acceptor atoms
		18	3D	MPSCAA-3	Sum of (surface area * charges) on acceptor atoms / total molecular surface area
		19	2D	MPCDTH	Count of donated hydrogens
		20	2D	MPCTAA	Count of acceptor atoms
		21	2D	MPMCHG	Max. charge difference between donor and acceptor
		22	2D	MPACHG	Average charge difference between donor and acceptors
		23	2D	MPRDTA	Ratio of number donors to number acceptors
31	HBPURE	HYDROGEN BOND SPECIFIC DESCRIPTORS FOR PURE COMPOUNDS			
		1		PSADH-1	Sum of surface area on donated hydrogens

		2		PSADH-2	Sum of surface area on donated hydrogens / number of donated hydrogens
		3		PSADH-3	Sum of surface area on donated hydrogens / total molecular surface area
		4	2D	PCHDH-1	Sum of charges on all donated hydrogens
		5	2D	PCHDH-2	Sum of charges on all donated hydrogens / number of donated hydrogens
		6		PCHDH-3	Sum of charges on all donated hydrogens / total molecular surface area
		7		PSCDH-1	Sum of (surface area * charges) on donated hydrogens
		8		PSCDH-2	Sum of charges on donated hydrogens / number of donated hydrogens
		9		PSCDH-3	Sum of (surface area * charges) on donated hydrogens / total molecular surface area
		10		PSAAA-1	Sum of surface area on acceptor atoms
		11		PSAAA-2	Sum of surface area on acceptor atoms / number of acceptor atoms
		12		PSAAA-3	Sum of surface area on acceptor atoms / total molecular surface area
		13	2D	PCHAA-1	Sum of charges on acceptor atoms
		14	2D	PCHAA-2	Sum of charges on acceptor atoms / number of acceptor atoms
		15		PCHAA-3	Sum of charges on acceptor atoms / total molecular surface area
		16		PSCAA-1	Sum of (surface area * charges) on acceptor atoms
		17		PSCAA-2	Sum of (surface area * charges) on acceptor atoms / number of acceptor atoms
		18		PSCAA-3	Sum of (surface area * charges) on acceptor atoms / total molecular surface area
		19	2D	PCDTH	Count of donated hydrogens
		20	2D	PCTAA	Count of acceptor atoms
		21	2D	PMCHG	Max. charge difference between donor and acceptor
		22	2D	PACHG	Average charge difference between donor and acceptor
		23	2D	PRDTA	Ratio of number donors to number acceptors
32	HMO	HUCKEL MOLECULAR ORBITAL CALCULATIONS			
		1	2D	AMPN	Minimum autopolarizability value
		2	2D	APMX	Maximum autopolarizability value
		3	2D	BOMN	Minimum bond order
		4	2D	BOMX	Maximum bond order

		5	2D	EDMN	Minimum electron density value
		6	2D	EDMX	Maximum electron density value
		7	2D	HOMO	Highest occupied molecular orbital
		8	2D	LUMO	Lowest unoccupied molecular orbital
		9	2D	ETOT	Total energy
		10	2D	FVMN	Minimum free valence value
		11	2D	FVMX	Maximum free valence value
		12	2D	SEMN	Min. electrophilic superdelocalizability
		13	2D	SEMX	Max. electrophilic superdelocalizability
		14	2D	SNMN	Min. nucleophilic superdelocalizability
		15	2D	SNMX	Max. nucleophilic superdelocalizability
		16	2D	SRMN	Min. free radical superdelocalizability
		17	2D	SRMX	Max. free radical superdelocalizability
33	LOVERB	LENGTH-TO-BREADTH RATIO			
		1	3D	L/B1	Length-to-breath ration (Maximum L/B)
		2	3D	L/B2	Length-to-breath ration (Minimum area)
	LEADLIKENESS				
		1	2D	DC_LEADL	Donors count
		2	2D	CNO_LEADL	Count of NO
		3	2D	MW_LEADL	Mass
		4	2D	RC_LEADL	Rings count
		5	2D	CRB_LEADL	Count of rotatable bonds
		6	2D	FQLOGP	FQLogP
		7	2D	FQLOGS	FQLogS
34	MlogP				
		1	2D	MLOGP	Calclate of LogP(Moriguchi, Hirono)
35	MOPAC	MOPAC7 Descriptor			
		1	3D	HF	Heat of Formation
		2	3D	DIP	Dipole Moment
		3	3D	DIPX	Dipole Moment X
		4	3D	DIPY	Dipole Moment Y
		5	3D	DIPZ	Dipole Moment Z
		6	3D	HOMO	HOMO Energy
		7	3D	LUMO	LUMO Energy
		8	3D	ENEG	Electronegativity
		9	3D	HARD	Hardness

		10	3D	PCHGN	Most negative partial charge
		11	3D	PCHGP	Most positive partial charge
		12	3D	PCHGNH	Most negative partial charge on H atom
		13	3D	PCHGMH	Mean partial charge on H atoms
		14	3D	PCHGPH	Most positive partial charge on H atom
		15	3D	PCHGNC	Most negative partial charge on C atom
		16	3D	PCHGMC	Mean partial charge on C atoms
		17	3D	PCHGPC	Most positive partial charge on C atom
		18	3D	PCHGNN	Most negative partial charge on N atom
		19	3D	PCHGMN	Mean partial charge on N atoms
		20	3D	PCHGPN	Most positive partial charge on N atom
		21	3D	PCHGNO	Most negative partial charge on O atom
		22	3D	PCHGMO	Mean partial charge on O atoms
		23	3D	PCHGPO	Most positive partial charge on O atom
		24	3D	PCHGNX	Most negative partial charge on Halogen atom
		25	3D	PCHGMX	Mean partial charge on Halogen atoms
		26	3D	PCHGPX	Most positive partial charge on Halogen atom
		27	3D	PCHGHT	Most negative partial charge on heteroatom
		28	3D	PCHGMHT	Mean partial charge on heteroatoms
		29	3D	PCHGPHT	Most positive partial on heteroatom
36	MPOLR	MOLECULAR POLARIZABILITY CALCULATION			
		1	2D	MPOL	Molecular polarizability
37	MRFRAC	MOLAR REFRACTION CALCULATION			
		1	2D	MREF	Molar refractivity
38	SAVOL	SURFACE AREA AND VOLUME CALCULATION			
		1	3D	SA	Pearlman excluded surface area for solvent radius of (*/100)
		2	3D	VOL	Pearlman excluded volume for solvent radius of (*/100)
39	SHADOW	CALCULATION OF SHADOW AREAS			
		1	3D	SHDW1	Shadow area 1 (XY plane)
		2	3D	SHDW2	Shadow area 2 (XZ plane)
		3	3D	SHDW3	Shadow area 3 (YZ plane)
		4	3D	SHDW4	Shadow area 4 (normalized SHDW1)
		5	3D	SHDW5	Shadow area 5 (normalized SHDW2)
		6	3D	SHDW6	Shadow area 6 (normalized SHDW3)
40	STRAIN	MOLECULAR STRAIN ENERGY CALCULATIONS			
		1	3D	STRA1	Angle strain energy of molecule
		2	3D	STRA2	Bond strain energy of molecule

		3	3D	STRA3	Non-bonded strain energy of molecule
		4	3D	STRA4	Torsional strain energy of molecule
		5	3D	STRA5	Other strain energy of molecule
		6	3D	STRA6	Total strain energy of molecule
41	TPSA	Topological Polar Surface Area			
		1	2D	TPSA	Topological Polar Surface Area