

MOLINSTINCTS

Technical Specification





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1. Available Pure Compounds Categorized by Database Product Number

Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
Enterprise				
Enterprise	All compounds available in MOLINSTINCTS	0 – 57		2,512,391
Free Radicals				
DB #01	• Free Radicals*	1 – 23	Compounds in DB #02 and #03 (= DB #02 + DB #03)	384,565
DB #02	▶ Hydrocarbon Radicals	1 – 23	Hydrocarbon radicals	284,033
DB #03	▶ Hetero Radicals	1 – 10	Hetero Radicals 1 - 10 Hetero (including atoms other than C and H) radicals	100,532
Hydrocarbons				
DB #04	• Hydrocarbons	1 – 57	Compounds in DB #05 – #09 (= DB #05 + DB #06 + DB #07 + DB #08 + DB #09)	949,509
DB #05	▶ Alkane	1 – 57	Alkane (Paraffin)	212,173
DB #06	▶ Alkene	2 – 30	Alkene (Olefin)	246,612
DB #07	▶ Alkyne	2 – 28	Alkyne	77,499
DB #08	▶ Cyclo-Hydrocarbons	3 – 57	Cycloalkane(Cycloparaffins, Naphthenes), Cycloalkene(Cycloolefins), Cycloalkylene	165,406
DB #09	▶ Aromatics	4 – 57	Aromatics	247,819
Hetero Compounds				
DB #10	• Hetero Compounds	0 – 57	Compounds in DB #11 – #17 (= DB #11 + DB #12 + DB #13 + DB #14 + DB #15 + DB #16 + DB #17)	1,178,318
DB #11	▶ O-Hetero Compounds	0 – 57	O-heterocyclic, carbonyl compound, aldehyde, ketone, ketene, carbonyl hydrate, hemiacetal, acetal, enol, enoether, hydroxy compound, alcohol, prim. alcohol, sec. alcohol, tert. alcohol, 1,2-diol, phenol, 1,2-diphenol, enediol, ether, dialkylether, alkylarylether, diarylether, peroxide, hydroperoxide, carboxylic acid, carboxylic acid ester, lactone, carboxylic acid anhydride, carbonic acid monoester, carbonic acid diester, alpha-hydroxyacid, carboxylic acid deriv., carbonic acid deriv.	172,417

* Note: Due to the unstable nature of radical compounds, some thermo-physico-chemical properties and molecular information are unavailable.
Total number of sets of information per radical compound is around 380.



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
DB #12	► N-Hetero Compounds	0 – 54	N-heterocyclic, imine, hydrazone, aminal, enamine, hydrazine derivative, amine, prim. amine, prim. aliphatic amine, prim. aromatic amine, sec. amine, sec. aliphatic amine, sec. mixed amine (aryl alkyl), sec. aromatic amine, tert. amine, tert. aliphatic amine, tert. mixed amine, tert. aromatic amine, carboxylic acid amidine, carboxylic acid amidrazone, nitrile, guanidine, azide, azo compound, cyanate, carbodiimide	100,541
DB #13	► S-Hetero Compounds	0 – 56	S-heterocyclic, thiocarbonyl compound, thioacetal, thioether, disulfide, thiocarboxylic acid deriv., thiol, alkylthiol, arylthiol, thiocarbonic acid deriv., sulfenic acid deriv., thiocarboxylic acid, thiocarboxylic acid ester, thiolactone	57,560
DB #14	► O/N-Hetero Compounds	0 – 38	semicarbazone, oxime, oxime ether, oxime, oxime ether, hemiaminal, 1,2-aminoalcohol, hydroxylamine, carboxylic acid amide, carboxylic acid prim. amide, carboxylic acid sec. amide, carboxylic acid tert. amide, lactam, carboxylic acid hydrazide, carboxylic acid azide, hydroxamic acid, acyl cyanide, imido ester, oxohetarene, carboxylic acid amide acetal, carboxylic acid imide, carboxylic acid unsubst. imide, carboxylic acid subst. imide, urea, isourea, semicarbazide, isocyanate, nitroso compound, nitro compound, nitrite, nitrate, alpha-aminoacid	374,423
DB #15	► O/S-Hetero Compounds	0 – 36	thiocarbonic acid monoester, thiocarbonic acid diester, sulfuric acid monoester, sulfuric acid diester, sulfonic acid, sulfonic acid ester, sulfone, sulfoxide, sulfenic acid, sulfinic acid ester, sulfinic acid ester, sulfinic acid ester, sulfuric acid deriv., sulfonic acid deriv., sulfinic acid deriv.	76,083
DB #16	► N/S-Hetero Compounds	0 – 25	thiosemicarbazone, thiohemiaminal, thiolactam, imidothioester, thioxohetarene, thiourea, isothiurea, thiosemicarbazide, thiocyanate, isothiocyanate, thiocarbamic acid deriv.	112,136
DB #17	► N/O/S-Hetero Compounds	0 – 32	thiocarbamic acid, thiocarbamic acid ester, sulfuric acid amide ester, sulfuric acid amide, sulfuric acid diamide, sulfonamide, sulfinic acid amide	285,158
Fuels				
DB #18	Gasoline	5 – 12	Alkane, Cycloalkane	104,681
DB #19	Jet-fuel	10 – 15	Alkane, Aromatics	170,810
DB #20	Diesel	12 – 25	Alkane, Alkene, Cycloalkane, Aromatics	731,935
DB #21	Bio-Diesel	12 – 19	Alkane, Alkene, Cycloalkane, Aromatics	669,038



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
Chemical Process related Compounds				
DB #22	Thermal Cracking	1 – 15	Alkane, Alkene, Alkyne, Aromatics, Hydrocarbon radicals	488,997
DB #23	Catalytic Cracking	1 – 40	Alkane, Alkene, Aromatics, Cycloalkane	791,485
DB #24	Hydro Cracking	5 – 19	Alkane, Cycloalkane, Aromatics, Hydrocarbon radicals	764,759
DB #25	Desulfurization	1 – 20	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics, alcohol, ether, ketone, aldehyde, carboxylic acid, carboxylic acid ester, N-heterocyclic, S-heterocyclic, Hetero radicals	984,196
DB #26	Isomerization	4 – 15	Alkane, Alkene, Aromatics	230,014
DB #27	Catalytic Reforming	6 – 15	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics	404,641
DB #28	Combustion	1 – 24	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics, Hydrocarbon radicals, Hetero radicals, alcohol, ether, ketone, aldehyde, carboxylic acid, carboxylic acid ester, N-heterocyclic, S-heterocyclic	1,298,757
DB #29	Soot	13 – 24	Aromatics	245,098
DB #30	Naphtha	1 – 15	Alkane, Alkene, Alkyne, Aromatics	271,238
DB #31	Gas-To-Liquid (GTL, CH ₄ Reforming + Fischer-Tropsch)	1 – 57	Parafin, Cyclo-parafin, Olefin, Cyclo-olefin, Diene, Aromatics, Alcohol, Phenol, Aldehyde, Carboxylic acid, Ester, Ketone, Acetal, Ether, Furan	843,809
DB #32	Coal-To-Liquid (CTL, Coal Gasification + Fischer-Tropsch)	1 – 57	Parafin, Cyclo-parafin, Olefin, Cyclo-olefin, Diene, Aromatics, Alcohol, Phenol, Aldehyde, Carboxylic acid, Ester, Ketone, Acetal, Ether, Furan, Pyran, Pridine, Indole, Quinoline, Aniline, Nitrile, Phenazine, Carbazole, Thiophene, Hydrocarbon Radicals, Hetero Radicals	1,234,093
DB #33	Methanol-To-Olefin (MTO) / Methanol-To-Gasoline (MTG)	1 – 57	Parafin, Olefin, Aromatics, Methanol, Dimethyl Ether, Water	682,041



Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
Drug-like Compounds				
DB #34	Drug-like Compounds	1 - 57	aldehyde, ketone, oxime, oxime ether, ketene acetal derivative, carbonyl hydrate, hemiacetal, acetal, enol, enolether, alcohol, prim. alcohol, sec. alcohol, tert. alcohol, phenol, enediol, ether, dialkylether, alkylarylether, diarylether, peroxide, hydroperoxide, carboxylic acid, carboxylic acid ester, lactone, orthocarboxylic acid deriv., carboxylic acid orthoester, carboxylic acid anhydride, carbonic acid deriv., carbonic acid monoester, carbonic acid diester, alpha-hydroxyacid, imine, hydrazone, semicarbazone, thiosemicarbazone, aminal, enamine, hydrazine derivative, amine, prim. amine, prim. aliphatic amine, prim. aromatic amine, sec. amine, sec. aliphatic amine, sec. mixed amine (aryl alkyl), sec. aromatic amine, tert. amine, tert. aliphatic amine, tert. mixed amine, tert. aromatic amine, nitrile, acyl cyanide, iminoheterene, guanidine, thiosemicarbazide, azide, azo compound, carbodiimide, thioaldehyde, thioketone, thioacetal, thioether, disulfide, alkylthiol, arylthiol, sulfurous acid deriv, hemiaminal, hydroxylamine, carboxylic acid prim. amide, carboxylic acid sec. amide, carboxylic acid tert. amide, lactam, carboxylic acid hydrazide, hydroxamic acid, carboxylic acid amidine, carboxylic acid amidrazone, imido ester, oxoheterene, carboxylic acid amide acetal, carboxylic acid unsubst. imide, carboxylic acid subst. imide, carbamic acid deriv, carbamic acid, carbamic acid ester (urethane), urea, isourea, semicarbazide, cyanate, isocyanate, nitroso compound, nitro compound, nitrite, nitrate, alpha-aminoacid, thiohemiaminal, imidothioester, thioxoheterene, thiocyanate, isothiocyanate, thiocarboxylic acid, thiocarboxylic acid ester, thiolactone, thiocarboxylic acid amide, thiolactam, thiocarbonic acid deriv., thiocarbonic acid monoester, thiocarbonic acid diester, thiourea, isothiurea, sulfuric acid deriv., sulfuric acid monoester, sulfuric acid diester, sulfonic acid deriv., sulfonic acid, sulfonic acid ester, sulfone, sulfoxide, sulfinic acid deriv., sulfinic acid, sulfinic acid ester, sulfenic acid deriv., sulfenic acid, sulfenic acid ester, thiocarbamic acid deriv., thiocarbamic acid, thiocarbamic acid ester, sulfuric acid amide ester, sulfuric acid amide, sulfuric acid diamide, sulfonamide, sulfinic acid amide, sulfenic acid amide	1,050,384



2. Available Properties & Molecular Information per compound

2.1. Compound Identification

1	2D Structure	4	Molecular Weight
2	Formula	5	InChI
3	IUPAC Name		

2.2. Thermo-Physico-Chemical Properties (constant)

1	Absolute Entropy of Ideal Gas at 298.15 K and 1 bar	19	Standard State Enthalpy of Formation at 298.15 K and 1 bar
2	Acentric Factor	20	Standard State Gibbs Energy of Formation at 298.15 K and 1 bar
3	Critical Compressibility Factor	21	Van Der Waals Area
4	Critical Pressure	22	Van Der Waals Reduced Volume
5	Critical Temperature	23	Magnetic Susceptibility
6	Critical Volume	24	Polarizability
7	Dipole Moment	25	Ionization Potential
8	Enthalpy of Formation for Ideal Gas at 298.15 K	26	Electron affinity
9	Enthalpy of Fusion at Melting Point	27	Flash Point
10	Gibbs Energy of Formation for Ideal Gas at 298.15 K and 1 bar	28	Parachor
11	Liquid Molar Volume at 298.15 K(1/LDE298)	29	Lower Flammability Limit Temperature
12	Molecular Weight	30	Lower Flammability Limit Volume Percent
13	Net Standard State Enthalpy of Combustion at 298.15 K	31	Upper Flammability Limit Temperature
14	Normal Boiling Point	32	Upper Flammability Limit Volume Percent
15	Radius of Gyration	33	Liquid Density at Normal Boiling Point
16	Refractive Index	34	Heat of Vaporization at 298.15K



2.2. Thermo-Physico-Chemical Properties (constant)

17	Solubility Parameter at 298.15 K	35	Heat of Vaporization at Normal Boiling Point
18	Standard State Absolute Entropy at 298.15 K and 1 bar		

2.3. Thermo-Physico-Chemical Properties (temperature-dependent)

1	Heat Capacity of Ideal Gas	6	Thermal Conductivity of Liquid
2	Heat Capacity of Liquid	7	Thermal Conductivity of Gas
3	Heat of Vaporization	8	Vapor Pressure of Liquid
4	Liquid Density	9	Viscosity of Liquid
5	Surface Tension	10	Viscosity of Gas
		11	Second Virial Coefficient

2.4. Quantum Information

1	Atoms	11	Primitive Shells
2	Charge	12	Virial Ratio
3	Multiplicity	13	Total Energy
4	Electrons	14	Atomic Numbers
5	Alpha electrons	15	Nuclear Charges
6	Beta electrons	16	Cartesian Coord.
7	Basis functions	17	Cartesian Gradient
8	Contracted Shells	18	Cartesian Force Constants
9	Highest Angular Momentum	19	Dipole Moment
10	Largest Deg. of Contraction	20	Mulliken Charges



2.5. Molecular descriptors

2.5.1. Molecular descriptors : Constitutional descriptors

1	Number of atoms	30	number of non-H atoms
2	Relative number of C atoms	31	number of bonds
3	Relative number of H atoms	32	number of non-H bonds
4	Relative number of O atoms	33	number of multiple bonds
5	Relative number of N atoms	34	sum of conventional bond orders (H-depleted)
6	Relative number of S atoms	35	aromatic ratio
7	Number of single bonds	36	number of rings
8	Relative number of single bonds	37	number of circuits
9	Relative number of double bonds	38	number of rotatable bonds
10	Relative number of triple bonds	39	rotatable bond fraction
11	Number of aromatic bonds	40	number of double bonds
12	Relative number of aromatic bonds	41	number of triple bonds
13	Relative number of rings	42	number of conjugated bonds
14	Relative number of benzene rings	43	number of Hydrogen atoms
15	Molecular weight	44	number of Carbon atoms
16	Relative molecular weight	45	number of Nitrogen atoms
17	Gravitation index (all bonds)	46	number of Oxygen atoms
18	Gravitation index (all pairs)	47	number of Sulfur atoms
19	Cubic root of Gravitation index (all bonds)	48	number of 3-membered rings
20	Cubic root of Gravitation index (all pairs)	49	number of 4-membered rings
21	average molecular weight	50	number of 5-membered rings
22	sum of atomic van der Waals volumes (scaled on Carbon atom)	51	number of 6-membered rings
23	sum of atomic Sanderson electronegativities (scaled on Carbon atom)	52	number of 7-membered rings



2.5.1. Molecular descriptors : Constitutional descriptors

24	sum of atomic polarizabilities (scaled on Carbon atom)	53	number of 8-membered rings
25	sum of Kier-Hall electrotopological states	54	number of 9-membered rings
26	mean atomic van der Waals volume (scaled on Carbon atom)	55	number of 10-membered rings
27	mean atomic Sanderson electronegativity (scaled on Carbon atom)	56	number of 11-membered rings
28	mean atomic polarizability (scaled on Carbon atom)	57	number of 12-membered rings
29	mean electrotopological state	58	number of benzene-like rings

2.5.2. Molecular descriptors : Topological descriptors

1	Kier molecular flexibility index	58	detour index
2	Average Information content (order 0)	59	hyper-detour index
3	Average Information content (order 1)	60	reciprocal hyper-detour index
4	Average Information content (order 2)	61	distance/detour index
5	Information content (order 0)	62	all-path Wiener index
6	Information content (order 1)	63	Wiener-type index (Barysz distance matrix)
7	Information content (order 2)	64	Wiener-type index (mass weighted distance matrix)
8	Average Structural Information content (order 0)	65	Wiener-type index (van der Waals weighted distance matrix)
9	Average Structural Information content (order 1)	66	Wiener-type index (electronegativity weighted distance matrix)
10	Average Structural Information content (order 2)	67	Wiener-type index (polarizability weighted distance matrix)
11	Structural Information content (order 0)	68	Balaban distance connectivity index
12	Structural Information content (order 1)	69	Balaban-type index (Barysz distance matrix)
13	Structural Information content (order 2)	70	Balaban-type index (mass weighted distance matrix)
14	Average Complementary Information content (order 0)	71	Balaban-type index (van der Waals weighted distance matrix)
15	Average Complementary Information content (order 1)	72	Balaban-type index (electronegativity weighted distance matrix)
16	Average Complementary Information content (order 2)	73	Balaban-type index (polarizability weighted distance matrix)



2.5.2. Molecular descriptors : Topological descriptors

17	Complementary Information content (order 0)	74	maximal electrotopological negative variation
18	Complementary Information content (order 1)	75	maximal electrotopological positive variation
19	Complementary Information content (order 2)	76	molecular electrotopological variation
20	Average Bonding Information content (order 0)	77	electrotopological state topological parameter
21	Average Bonding Information content (order 1)	78	Kier symmetry index
22	Average Bonding Information content (order 2)	79	Kier alpha-modified shape index m1
23	Bonding Information content (order 0)	80	Kier alpha-modified shape index m2
24	Bonding Information content (order 1)	81	Kier alpha-modified shape index m3
25	Bonding Information content (order 2)	82	Kier benzene-likeness index
26	Balaban index	83	path/walk shape index m2
27	first Zagreb index M1	84	path/walk shape index m3
28	first Zagreb index by valence vertex degrees	85	path/walk shape index m4
29	second Zagreb index M2	86	path/walk shape index m5
30	second Zagreb index by valence vertex degrees	87	2D Petitjean shape index
31	Quadratic index	88	eccentric connectivity index
32	Narumi simple topological index (log S)	89	eccentricity
33	Narumi harmonic topological index (H)	90	average eccentricity
34	Narumi geometric topological index (G)	91	eccentric
35	Total structure connectivity index	92	mean distance degree deviation
36	Pogliani index	93	unipolarity
37	ramification index	94	centralization
38	polarity number	95	variation
39	log of product of row sums (PRS index)	96	Balaban centric index
40	average vertex distance degree	97	Lopping centric information index
41	mean square distance index (Balaban)	98	radial centric information index



2.5.2. Molecular descriptors : Topological descriptors

42	Schultz Molecular Topological Index	99	distance/detour ring index (order 3)
43	Schultz Molecular Topological Index by valence vertex degrees	100	distance/detour ring index (order 4)
44	Gutman Molecular Topological Index	101	distance/detour ring index (order 5)
45	Gutman Molecular Topological Index by valence vertex degrees	102	distance/detour ring index (order 6)
46	Xu index	103	distance/detour ring index (order 7)
47	superpendentic index	104	distance/detour ring index (order 8)
48	Wiener W index	105	distance/detour ring index (order 9)
49	mean Wiener index	106	distance/detour ring index (order 10)
50	Harary H index	107	distance/detour ring index (order 11)
51	square reciprocal distance sum index	108	distance/detour ring index (order 12)
52	quasi-Wiener index	109	sum of topological distances between N..N
53	first Mohar index TI1	110	sum of topological distances between N..O
54	second Mohar index TI2	111	sum of topological distances between N..S
55	spanning tree number (log)	112	sum of topological distances between O..O
56	hyper-distance-path index	113	sum of topological distances between O..S
57	reciprocal hyper-distance-path index	114	sum of topological distances between S..S

2.5.3. Molecular descriptors : Walk and path counts

1	molecular walk count k1	25	molecular path count m4
2	molecular walk count k2	26	molecular path count m5
3	molecular walk count k3	27	molecular path count m6
4	molecular walk count k4	28	molecular path count m7
5	molecular walk count k5	29	molecular path count m8
6	molecular walk count k6	30	molecular path count m9



2.5.3. Molecular descriptors : Walk and path counts

7	molecular walk count k7	31	molecular path count m10
8	molecular walk count k8	32	molecular multiple path count m1
9	molecular walk count k9	33	molecular multiple path count m2
10	molecular walk count k10	34	molecular multiple path count m3
11	total walk count	35	molecular multiple path count m4
12	self-returning walk count k1	36	molecular multiple path count m5
13	self-returning walk count k2	37	molecular multiple path count m6
14	self-returning walk count k3	38	molecular multiple path count m7
15	self-returning walk count k4	39	molecular multiple path count m8
16	self-returning walk count k5	40	molecular multiple path count m9
17	self-returning walk count k6	41	molecular multiple path count m10
18	self-returning walk count k7	42	total path count
19	self-returning walk count k8	43	conventional bond-order ID number
20	self-returning walk count k9	44	ratio of multiple path count over path count
21	self-returning walk count k10	45	difference between multiple path count and path count
22	molecular path count m1	46	Randic Connectivity ID number
23	molecular path count m2	47	Balaban ID number
24	molecular path count m3		

2.5.4. Molecular descriptors : Connectivity indices

1	connectivity index m0	18	valence connectivity index m5
2	connectivity index m1	19	avg valence connectivity index m0
3	connectivity index m2	20	avg valence connectivity index m1
4	connectivity index m3	21	avg valence connectivity index m2



2.5.4. Molecular descriptors : Connectivity indices

5	connectivity index m4	22	avg valence connectivity index m3
6	connectivity index m5	23	avg valence connectivity index m4
7	avg connectivity index m0	24	avg valence connectivity index m5
8	avg connectivity index m1	25	solvation connectivity index m0
9	avg connectivity index m2	26	solvation connectivity index m1
10	avg connectivity index m3	27	solvation connectivity index m2
11	avg connectivity index m4	28	solvation connectivity index m3
12	avg connectivity index m5	29	solvation connectivity index m4
13	valence connectivity index m0	30	solvation connectivity index m5
14	valence connectivity index m1	31	modified Randic connectivity index
15	valence connectivity index m2	32	reciprocal distance Randic-type index
16	valence connectivity index m3	33	reciprocal distance squared Randic-type index
17	valence connectivity index m4		

2.5.5. Molecular descriptors : Information indices

1	information index on molecular size	25	structural information content level1
2	total information index of atomic composition	26	complementary information content level1
3	mean information index on atomic composition	27	bond information content level1
4	mean information content on the distance equality	28	information content index level2
5	mean information content on the distance magnitude	29	total information content index level2
6	mean information content on the distance degree equality	30	structural information content level2
7	mean information content on the distance degree magnitude	31	complementary information content level2
8	total information content on the distance equality	32	bond information content level2
9	total information content on the distance magnitude	33	information content index level3



2.5.5. Molecular descriptors : Information indices

10	mean information content on the vertex degree equality	34	total information content index level3
11	mean information content on the vertex degree magnitude	35	structural information content level3
12	graph vertex complexity index	36	complementary information content level3
13	graph distance complexity index (log)	37	bond information content level3
14	Balaban U index	38	information content index level4
15	Balaban V index	39	total information content index level4
16	Balaban X index	40	structural information content level4
17	Balaban Y index	41	complementary information content level4
18	information content index level0	42	bond information content level4
19	total information content index level0	43	information content index level5
20	structural information content level0	44	total information content index level5
21	complementary information content level0	45	structural information content level5
22	bond information content level0	46	complementary information content level5
23	information content index level1	47	bond information content level5
24	total information content index level1		

2.5.6. Molecular descriptors : List of 2D autocorrelation indices

1	Broto-Moreau autocorrelation d1 (atomic masses)	49	Moran autocorrelation d1 (atomic Sanderson electronegativities)
2	Broto-Moreau autocorrelation d2 (atomic masses)	50	Moran autocorrelation d2 (atomic Sanderson electronegativities)
3	Broto-Moreau autocorrelation d3 (atomic masses)	51	Moran autocorrelation d3 (atomic Sanderson electronegativities)
4	Broto-Moreau autocorrelation d4 (atomic masses)	52	Moran autocorrelation d4 (atomic Sanderson electronegativities)
5	Broto-Moreau autocorrelation d5 (atomic masses)	53	Moran autocorrelation d5 (atomic Sanderson electronegativities)
6	Broto-Moreau autocorrelation d6 (atomic masses)	54	Moran autocorrelation d6 (atomic Sanderson electronegativities)
7	Broto-Moreau autocorrelation d7 (atomic masses)	55	Moran autocorrelation d7 (atomic Sanderson electronegativities)



2.5.6. Molecular descriptors : List of 2D autocorrelation indices

8	Broto-Moreau autocorrelation d8 (atomic masses)	56	Moran autocorrelation d8 (atomic Sanderson electronegativities)
9	Broto-Moreau autocorrelation d1 (atomic van der Waals volumes)	57	Moran autocorrelation d1 (atomic polarizabilities)
10	Broto-Moreau autocorrelation d2 (atomic van der Waals volumes)	58	Moran autocorrelation d2 (atomic polarizabilities)
11	Broto-Moreau autocorrelation d3 (atomic van der Waals volumes)	59	Moran autocorrelation d3 (atomic polarizabilities)
12	Broto-Moreau autocorrelation d4 (atomic van der Waals volumes)	60	Moran autocorrelation d4 (atomic polarizabilities)
13	Broto-Moreau autocorrelation d5 (atomic van der Waals volumes)	61	Moran autocorrelation d5 (atomic polarizabilities)
14	Broto-Moreau autocorrelation d6 (atomic van der Waals volumes)	62	Moran autocorrelation d6 (atomic polarizabilities)
15	Broto-Moreau autocorrelation d7 (atomic van der Waals volumes)	63	Moran autocorrelation d7 (atomic polarizabilities)
16	Broto-Moreau autocorrelation d8 (atomic van der Waals volumes)	64	Moran autocorrelation d8 (atomic polarizabilities)
17	Broto-Moreau autocorrelation d1 (atomic Sanderson electronegativities)	65	Geary autocorrelation d1 (atomic masses)
18	Broto-Moreau autocorrelation d2 (atomic Sanderson electronegativities)	66	Geary autocorrelation d2 (atomic masses)
19	Broto-Moreau autocorrelation d3 (atomic Sanderson electronegativities)	67	Geary autocorrelation d3 (atomic masses)
20	Broto-Moreau autocorrelation d4 (atomic Sanderson electronegativities)	68	Geary autocorrelation d4 (atomic masses)
21	Broto-Moreau autocorrelation d5 (atomic Sanderson electronegativities)	69	Geary autocorrelation d5 (atomic masses)
22	Broto-Moreau autocorrelation d6 (atomic Sanderson electronegativities)	70	Geary autocorrelation d6 (atomic masses)
23	Broto-Moreau autocorrelation d7 (atomic Sanderson electronegativities)	71	Geary autocorrelation d7 (atomic masses)
24	Broto-Moreau autocorrelation d8 (atomic Sanderson electronegativities)	72	Geary autocorrelation d8 (atomic masses)
25	Broto-Moreau autocorrelation d1 (atomic polarizabilities)	73	Geary autocorrelation d1 (atomic van der Waals volumes)
26	Broto-Moreau autocorrelation d2 (atomic polarizabilities)	74	Geary autocorrelation d2 (atomic van der Waals volumes)
27	Broto-Moreau autocorrelation d3 (atomic polarizabilities)	75	Geary autocorrelation d3 (atomic van der Waals volumes)
28	Broto-Moreau autocorrelation d4 (atomic polarizabilities)	76	Geary autocorrelation d4 (atomic van der Waals volumes)
29	Broto-Moreau autocorrelation d5 (atomic polarizabilities)	77	Geary autocorrelation d5 (atomic van der Waals volumes)
30	Broto-Moreau autocorrelation d6 (atomic polarizabilities)	78	Geary autocorrelation d6 (atomic van der Waals volumes)
31	Broto-Moreau autocorrelation d7 (atomic polarizabilities)	79	Geary autocorrelation d7 (atomic van der Waals volumes)
32	Broto-Moreau autocorrelation d8 (atomic polarizabilities)	80	Geary autocorrelation d8 (atomic van der Waals volumes)



2.5.6. Molecular descriptors : List of 2D autocorrelation indices

33	Moran autocorrelation d1 (atomic masses)	81	Geary autocorrelation d1 (atomic Sanderson electronegativities)
34	Moran autocorrelation d2 (atomic masses)	82	Geary autocorrelation d2 (atomic Sanderson electronegativities)
35	Moran autocorrelation d3 (atomic masses)	83	Geary autocorrelation d3 (atomic Sanderson electronegativities)
36	Moran autocorrelation d4 (atomic masses)	84	Geary autocorrelation d4 (atomic Sanderson electronegativities)
37	Moran autocorrelation d5 (atomic masses)	85	Geary autocorrelation d5 (atomic Sanderson electronegativities)
38	Moran autocorrelation d6 (atomic masses)	86	Geary autocorrelation d6 (atomic Sanderson electronegativities)
39	Moran autocorrelation d7 (atomic masses)	87	Geary autocorrelation d7 (atomic Sanderson electronegativities)
40	Moran autocorrelation d8 (atomic masses)	88	Geary autocorrelation d8 (atomic Sanderson electronegativities)
41	Moran autocorrelation d1 (atomic van der Waals volumes)	89	Geary autocorrelation d1 (atomic polarizabilities)
42	Moran autocorrelation d2 (atomic van der Waals volumes)	90	Geary autocorrelation d2 (atomic polarizabilities)
43	Moran autocorrelation d3 (atomic van der Waals volumes)	91	Geary autocorrelation d3 (atomic polarizabilities)
44	Moran autocorrelation d4 (atomic van der Waals volumes)	92	Geary autocorrelation d4 (atomic polarizabilities)
45	Moran autocorrelation d5 (atomic van der Waals volumes)	93	Geary autocorrelation d5 (atomic polarizabilities)
46	Moran autocorrelation d6 (atomic van der Waals volumes)	94	Geary autocorrelation d6 (atomic polarizabilities)
47	Moran autocorrelation d7 (atomic van der Waals volumes)	95	Geary autocorrelation d7 (atomic polarizabilities)
48	Moran autocorrelation d8 (atomic van der Waals volumes)	96	Geary autocorrelation d8 (atomic polarizabilities)

2.5.7. Molecular descriptors : Edge adjacency indices

1	edge connectivity index (order 0)	55	spectral moment 8 of edge adjacency matrix
2	edge connectivity index (order 1)	56	spectral moment 9 of edge adjacency matrix
3	eigenvalue 1 of edge adjacency matrix (edge degrees)	57	spectral moment 10 of edge adjacency matrix
4	eigenvalue 2 of edge adjacency matrix (edge degrees)	58	spectral moment 11 of edge adjacency matrix
5	eigenvalue 3 of edge adjacency matrix (edge degrees)	59	spectral moment 12 of edge adjacency matrix
6	eigenvalue 4 of edge adjacency matrix (edge degrees)	60	spectral moment 13 of edge adjacency matrix



2.5.7. Molecular descriptors : Edge adjacency indices

7	eigenvalue 5 of edge adjacency matrix (edge degrees)	61	spectral moment 14 of edge adjacency matrix
8	eigenvalue 6 of edge adjacency matrix (edge degrees)	62	spectral moment 15 of edge adjacency matrix
9	eigenvalue 7 of edge adjacency matrix (edge degrees)	63	spectral moment 1 of edge adjacency matrix (edge degrees)
10	eigenvalue 8 of edge adjacency matrix (edge degrees)	64	spectral moment 2 of edge adjacency matrix (edge degrees)
11	eigenvalue 9 of edge adjacency matrix (edge degrees)	65	spectral moment 3 of edge adjacency matrix (edge degrees)
12	eigenvalue 10 of edge adjacency matrix (edge degrees)	66	spectral moment 4 of edge adjacency matrix (edge degrees)
13	eigenvalue 11 of edge adjacency matrix (edge degrees)	67	spectral moment 5 of edge adjacency matrix (edge degrees)
14	eigenvalue 12 of edge adjacency matrix (edge degrees)	68	spectral moment 6 of edge adjacency matrix (edge degrees)
15	eigenvalue 13 of edge adjacency matrix (edge degrees)	69	spectral moment 7 of edge adjacency matrix (edge degrees)
16	eigenvalue 14 of edge adjacency matrix (edge degrees)	70	spectral moment 8 of edge adjacency matrix (edge degrees)
17	eigenvalue 15 of edge adjacency matrix (edge degrees)	71	spectral moment 9 of edge adjacency matrix (edge degrees)
18	eigenvalue 1 of edge adjacency matrix (dipole moments)	72	spectral moment 10 of edge adjacency matrix (edge degrees)
19	eigenvalue 2 of edge adjacency matrix (dipole moments)	73	spectral moment 11 of edge adjacency matrix (edge degrees)
20	eigenvalue 3 of edge adjacency matrix (dipole moments)	74	spectral moment 12 of edge adjacency matrix (edge degrees)
21	eigenvalue 4 of edge adjacency matrix (dipole moments)	75	spectral moment 13 of edge adjacency matrix (edge degrees)
22	eigenvalue 5 of edge adjacency matrix (dipole moments)	76	spectral moment 14 of edge adjacency matrix (edge degrees)
23	eigenvalue 6 of edge adjacency matrix (dipole moments)	77	spectral moment 15 of edge adjacency matrix (edge degrees)
24	eigenvalue 7 of edge adjacency matrix (dipole moments)	78	spectral moment 1 of edge adjacency matrix (dipole moments)
25	eigenvalue 8 of edge adjacency matrix (dipole moments)	79	spectral moment 2 of edge adjacency matrix (dipole moments)
26	eigenvalue 9 of edge adjacency matrix (dipole moments)	80	spectral moment 3 of edge adjacency matrix (dipole moments)
27	eigenvalue 10 of edge adjacency matrix (dipole moments)	81	spectral moment 4 of edge adjacency matrix (dipole moments)
28	eigenvalue 11 of edge adjacency matrix (dipole moments)	82	spectral moment 5 of edge adjacency matrix (dipole moments)
29	eigenvalue 12 of edge adjacency matrix (dipole moments)	83	spectral moment 6 of edge adjacency matrix (dipole moments)
30	eigenvalue 13 of edge adjacency matrix (dipole moments)	84	spectral moment 7 of edge adjacency matrix (dipole moments)
31	eigenvalue 14 of edge adjacency matrix (dipole moments)	85	spectral moment 8 of edge adjacency matrix (dipole moments)



2.5.7. Molecular descriptors : Edge adjacency indices

32	eigenvalue 15 of edge adjacency matrix (dipole moments)	86	spectral moment 9 of edge adjacency matrix (dipole moments)
33	eigenvalue 1 of edge adjacency matrix (resonance integrals)	87	spectral moment 10 of edge adjacency matrix (dipole moments)
34	eigenvalue 2 of edge adjacency matrix (resonance integrals)	88	spectral moment 11 of edge adjacency matrix (dipole moments)
35	eigenvalue 3 of edge adjacency matrix (resonance integrals)	89	spectral moment 12 of edge adjacency matrix (dipole moments)
36	eigenvalue 4 of edge adjacency matrix (resonance integrals)	90	spectral moment 13 of edge adjacency matrix (dipole moments)
37	eigenvalue 5 of edge adjacency matrix (resonance integrals)	91	spectral moment 14 of edge adjacency matrix (dipole moments)
38	eigenvalue 6 of edge adjacency matrix (resonance integrals)	92	spectral moment 15 of edge adjacency matrix (dipole moments)
39	eigenvalue 7 of edge adjacency matrix (resonance integrals)	93	spectral moment 1 of edge adjacency matrix (resonance integrals)
40	eigenvalue 8 of edge adjacency matrix (resonance integrals)	94	spectral moment 2 of edge adjacency matrix (resonance integrals)
41	eigenvalue 9 of edge adjacency matrix (resonance integrals)	95	spectral moment 3 of edge adjacency matrix (resonance integrals)
42	eigenvalue 10 of edge adjacency matrix (resonance integrals)	96	spectral moment 4 of edge adjacency matrix (resonance integrals)
43	eigenvalue 11 of edge adjacency matrix (resonance integrals)	97	spectral moment 5 of edge adjacency matrix (resonance integrals)
44	eigenvalue 12 of edge adjacency matrix (resonance integrals)	98	spectral moment 6 of edge adjacency matrix (resonance integrals)
45	eigenvalue 13 of edge adjacency matrix (resonance integrals)	99	spectral moment 7 of edge adjacency matrix (resonance integrals)
46	eigenvalue 14 of edge adjacency matrix (resonance integrals)	100	spectral moment 8 of edge adjacency matrix (resonance integrals)
47	eigenvalue 15 of edge adjacency matrix (resonance integrals)	101	spectral moment 9 of edge adjacency matrix (resonance integrals)
48	spectral moment 1 of edge adjacency matrix	102	spectral moment 10 of edge adjacency matrix (resonance integrals)
49	spectral moment 2 of edge adjacency matrix	103	spectral moment 11 of edge adjacency matrix (resonance integrals)
50	spectral moment 3 of edge adjacency matrix	104	spectral moment 12 of edge adjacency matrix (resonance integrals)
51	spectral moment 4 of edge adjacency matrix	105	spectral moment 13 of edge adjacency matrix (resonance integrals)
52	spectral moment 5 of edge adjacency matrix	106	spectral moment 14 of edge adjacency matrix (resonance integrals)
53	spectral moment 6 of edge adjacency matrix	107	spectral moment 15 of edge adjacency matrix (resonance integrals)
54	spectral moment 7 of edge adjacency matrix		



2.5.8. Molecular descriptors : Burden eigenvalues descriptors

1	highest positive eigenvalue k1 of Burden matrix (atomic masses)	33	highest positive eigenvalue k1 of Burden matrix(atomic Sanderson electronegativities)
2	highest positive eigenvalue k2 of Burden matrix (atomic masses)	34	highest positive eigenvalue k2 of Burden matrix(atomic Sanderson electronegativities)
3	highest positive eigenvalue k3 of Burden matrix (atomic masses)	35	highest positive eigenvalue k3 of Burden matrix(atomic Sanderson electronegativities)
4	highest positive eigenvalue k4 of Burden matrix (atomic masses)	36	highest positive eigenvalue k4 of Burden matrix(atomic Sanderson electronegativities)
5	highest positive eigenvalue k5 of Burden matrix (atomic masses)	37	highest positive eigenvalue k5 of Burden matrix(atomic Sanderson electronegativities)
6	highest positive eigenvalue k6 of Burden matrix (atomic masses)	38	highest positive eigenvalue k6 of Burden matrix(atomic Sanderson electronegativities)
7	highest positive eigenvalue k7 of Burden matrix (atomic masses)	39	highest positive eigenvalue k7 of Burden matrix(atomic Sanderson electronegativities)
8	highest positive eigenvalue k8 of Burden matrix (atomic masses)	40	highest positive eigenvalue k8 of Burden matrix(atomic Sanderson electronegativities)
9	lowest negative eigenvalue k1 of Burden matrix (atomic masses)	41	lowest negative eigenvalue k1 of Burden matrix(atomic Sanderson electronegativities)
10	lowest negative eigenvalue k2 of Burden matrix (atomic masses)	42	lowest negative eigenvalue k2 of Burden matrix(atomic Sanderson electronegativities)
11	lowest negative eigenvalue k3 of Burden matrix (atomic masses)	43	lowest negative eigenvalue k3 of Burden matrix(atomic Sanderson electronegativities)
12	lowest negative eigenvalue k4 of Burden matrix (atomic masses)	44	lowest negative eigenvalue k4 of Burden matrix(atomic Sanderson electronegativities)
13	lowest negative eigenvalue k5 of Burden matrix (atomic masses)	45	lowest negative eigenvalue k5 of Burden matrix(atomic Sanderson electronegativities)
14	lowest negative eigenvalue k6 of Burden matrix (atomic masses)	46	lowest negative eigenvalue k6 of Burden matrix(atomic Sanderson electronegativities)
15	lowest negative eigenvalue k7 of Burden matrix (atomic masses)	47	lowest negative eigenvalue k7 of Burden matrix(atomic Sanderson electronegativities)
16	lowest negative eigenvalue k8 of Burden matrix (atomic masses)	48	lowest negative eigenvalue k8 of Burden matrix(atomic Sanderson electronegativities)
17	highest positive eigenvalue k1 of Burden matrix (atomic van der Waals volumes)	49	highest positive eigenvalue k1 of Burden matrix (atomic polarizabilities)
18	highest positive eigenvalue k2 of Burden matrix (atomic van der Waals volumes)	50	highest positive eigenvalue k2 of Burden matrix (atomic polarizabilities)
19	highest positive eigenvalue k3 of Burden matrix (atomic van der Waals volumes)	51	highest positive eigenvalue k3 of Burden matrix (atomic polarizabilities)
20	highest positive eigenvalue k4 of Burden matrix (atomic van der Waals volumes)	52	highest positive eigenvalue k4 of Burden matrix (atomic polarizabilities)
21	highest positive eigenvalue k5 of Burden matrix (atomic van der Waals volumes)	53	highest positive eigenvalue k5 of Burden matrix (atomic polarizabilities)
22	highest positive eigenvalue k6 of Burden matrix (atomic van der Waals volumes)	54	highest positive eigenvalue k6 of Burden matrix (atomic polarizabilities)
23	highest positive eigenvalue k7 of Burden matrix (atomic van der Waals volumes)	55	highest positive eigenvalue k7 of Burden matrix (atomic polarizabilities)
24	highest positive eigenvalue k8 of Burden matrix (atomic van der Waals volumes)	56	highest positive eigenvalue k8 of Burden matrix (atomic polarizabilities)



2.5.8. Molecular descriptors : Burden eigenvalues descriptors

25	lowest negative eigenvalue k1 of Burden matrix (atomic van der Waals volumes)	57	lowest negative eigenvalue k1 of Burden matrix (atomic polarizabilities)
26	lowest negative eigenvalue k2 of Burden matrix (atomic van der Waals volumes)	58	lowest negative eigenvalue k2 of Burden matrix (atomic polarizabilities)
27	lowest negative eigenvalue k3 of Burden matrix (atomic van der Waals volumes)	59	lowest negative eigenvalue k3 of Burden matrix (atomic polarizabilities)
28	lowest negative eigenvalue k4 of Burden matrix (atomic van der Waals volumes)	60	lowest negative eigenvalue k4 of Burden matrix (atomic polarizabilities)
29	lowest negative eigenvalue k5 of Burden matrix (atomic van der Waals volumes)	61	lowest negative eigenvalue k5 of Burden matrix (atomic polarizabilities)
30	lowest negative eigenvalue k6 of Burden matrix (atomic van der Waals volumes)	62	lowest negative eigenvalue k6 of Burden matrix (atomic polarizabilities)
31	lowest negative eigenvalue k7 of Burden matrix (atomic van der Waals volumes)	63	lowest negative eigenvalue k7 of Burden matrix (atomic polarizabilities)
32	lowest negative eigenvalue k8 of Burden matrix (atomic van der Waals volumes)	64	lowest negative eigenvalue k8 of Burden matrix (atomic polarizabilities)

2.5.9. Molecular descriptors : Topological charge indices

1	topological charge index k1	12	mean topological charge index k2
2	topological charge index k2	13	mean topological charge index k3
3	topological charge index k3	14	mean topological charge index k4
4	topological charge index k4	15	mean topological charge index k5
5	topological charge index k5	16	mean topological charge index k6
6	topological charge index k6	17	mean topological charge index k7
7	topological charge index k7	18	mean topological charge index k8
8	topological charge index k8	19	mean topological charge index k9
9	topological charge index k9	20	mean topological charge index k10
10	topological charge index k10	21	global topological charge index
11	mean topological charge index k1		



2.5.10. Molecular descriptors : Eigenvalue-based indices

1	Lovasz-Pelikan index (leading eigenvalue)	23	Randic-type eigenvector coeff. sum (distance matrix)
2	leading eigenvalue (Barysz distance matrix)	24	avg Randic-type eigenvector-based index (distance matrix)
3	leading eigenvalue (mass weighted distance matrix)	25	eigenvector coeff. sum (Barysz distance matrix)
4	leading eigenvalue (van der Waals weighted distance matrix)	26	avg eigenvector coeff. sum (Barysz distance matrix)
5	leading eigenvalue (electronegativity weighted distance matrix)	27	Randic-type eigenvector coeff. sum (Barysz distance matrix)
6	leading eigenvalue (polarizability weighted distance matrix)	28	avg Randic-type eigenvector-based index (Barysz distance matrix)
7	eigenvalue sum (Barysz distance matrix)	29	eigenvector coeff. sum (mass weighted distance matrix)
8	eigenvalue sum (mass weighted distance matrix)	30	avg eigenvector coeff. sum (mass weighted distance matrix)
9	eigenvalue sum (van der Waals weighted distance matrix)	31	Randic-type eigenvector coeff. sum (mass weighted distance matrix)
10	eigenvalue sum (electronegativity weighted distance matrix)	32	avg Randic-type eigenvector-based index (mass weighted distance matrix)
11	eigenvalue sum (polarizability weighted distance matrix)	33	eigenvector coeff. sum (van der Waals weighted distance matrix)
12	abs. eigenvalue sum (Barysz distance matrix)	34	avg eigenvector coeff. sum (van der Waals weighted distance matrix)
13	abs. eigenvalue sum (mass weighted distance matrix)	35	Randic-type eigenvector coeff. sum (van der Waals weighted distance matrix)
14	abs. eigenvalue sum (van der Waals weighted distance matrix)	36	avg Randic-type eigenvector-based index (van der Waals weighted distance matrix)
15	abs. eigenvalue sum (electronegativity weighted distance matrix)	37	eigenvector coeff. sum (electronegativity weighted distance matrix)
16	abs. eigenvalue sum (polarizability weighted distance matrix)	38	avg eigenvector coeff. sum (electronegativity weighted distance matrix)
17	eigenvector coeff. sum (adjacency matrix)	39	Randic-type eigenvector coeff. sum (electronegativity weighted distance matrix)
18	avg eigenvector coeff. sum (adjacency matrix)	40	avg Randic-type eigenvector-based index (electronegativity weighted distance matrix)
19	Randic-type eigenvector coeff. sum (adjacency matrix)	41	eigenvector coeff. sum (polarizability weighted distance matrix)
20	avg Randic-type eigenvector-based index (adjacency matrix)	42	avg eigenvector coeff. sum (polarizability weighted distance matrix)



2.5.10. Molecular descriptors : Eigenvalue-based indices

21	eigenvector coeff. sum (distance matrix)	43	Randic-type eigenvector coeff. sum (polarizability weighted distance matrix)
22	avg eigenvector coeff. sum (distance matrix)	44	avg Randic-type eigenvector-based index (polarizability weighted distance matrix)

2.5.11. Molecular descriptors : Randic molecular profiles

1	Randic molecular profile k1	22	Randic shape profile k2
2	Randic molecular profile k2	23	Randic shape profile k3
3	Randic molecular profile k3	24	Randic shape profile k4
4	Randic molecular profile k4	25	Randic shape profile k5
5	Randic molecular profile k5	26	Randic shape profile k6
6	Randic molecular profile k6	27	Randic shape profile k7
7	Randic molecular profile k7	28	Randic shape profile k8
8	Randic molecular profile k8	29	Randic shape profile k9
9	Randic molecular profile k9	30	Randic shape profile k10
10	Randic molecular profile k10	31	Randic shape profile k11
11	Randic molecular profile k11	32	Randic shape profile k12
12	Randic molecular profile k12	33	Randic shape profile k13
13	Randic molecular profile k13	34	Randic shape profile k14
14	Randic molecular profile k14	35	Randic shape profile k15
15	Randic molecular profile k15	36	Randic shape profile k16
16	Randic molecular profile k16	37	Randic shape profile k17
17	Randic molecular profile k17	38	Randic shape profile k18
18	Randic molecular profile k18	39	Randic shape profile k19
19	Randic molecular profile k19	40	Randic shape profile k20



2.5.11. Molecular descriptors : Randic molecular profiles

20	Randic molecular profile k20	41	avg Randic shape profile index (order 2)
21	Randic shape profile k1		

2.5.12. Molecular descriptors : Geometrical descriptors

1	Moment of inertia A	29	Length / Breadth by WHIM
2	Moment of inertia B	30	absolute eigenvalue sum on geometry matrix
3	Moment of inertia C	31	Harmonic Oscillator Model of Aromaticity index
4	XY Shadow	32	Jug ring current index
5	XY Shadow / XY Rectangle	33	aromaticity index
6	YZ Shadow	34	Homeostasis Model Assessment (HOMA) total index
7	YZ Shadow / YZ Rectangle	35	CoMMA displacement (atomic masses)
8	ZX Shadow	36	CoMMA quadrupole xx (atomic masses)
9	ZX Shadow / ZX Rectangle	37	CoMMA quadrupole yy (atomic masses)
10	Molecular volume	38	CoMMA quadrupole zz (atomic masses)
11	Molecular volume / XYZ Box	39	CoMMA displacement (atomic van der Waals volumes)
12	Molecular surface area	40	CoMMA quadrupole xx (atomic van der Waals volumes)
13	3D-Wiener index	41	CoMMA quadrupole yy (atomic van der Waals volumes)
14	3D-Balaban index	42	CoMMA quadrupole zz (atomic van der Waals volumes)
15	3D-Harary index	43	CoMMA displacement (atomic Sanderson electronegativities)
16	average geometric distance degree	44	CoMMA quadrupole xx (atomic Sanderson electronegativities)
17	distance/distance index	45	CoMMA quadrupole yy (atomic Sanderson electronegativities)
18	average distance/distance degree	46	CoMMA quadrupole zz (atomic Sanderson electronegativities)
19	gravitational index G1	47	CoMMA displacement (atomic polarizabilities)
20	gravitational index G2 (bond-restricted)	48	CoMMA quadrupole xx (atomic polarizabilities)



2.5.12. Molecular descriptors : Geometrical descriptors

21	radius of gyration (mass weighted)	49	CoMMA quadrupole yy (atomic polarizabilities)
22	span R	50	CoMMA quadrupole zz (atomic polarizabilities)
23	average span R	51	sum of geometrical distances between N..N
24	molecular eccentricity	52	sum of geometrical distances between N..O
25	sphericity index	53	sum of geometrical distances between N..S
26	asphericity index	54	sum of geometrical distances between O..O
27	folding degree index	55	sum of geometrical distances between O..S
28	3D Petitjean shape index	56	sum of geometrical distances between S..S

2.5.13. Molecular descriptors : RDF descriptors

1	RDF s10 (unweighted)	76	RDF s85 (atomic van der Waals volumes)
2	RDF s15 (unweighted)	77	RDF s90 (atomic van der Waals volumes)
3	RDF s20 (unweighted)	78	RDF s95 (atomic van der Waals volumes)
4	RDF s25 (unweighted)	79	RDF s100 (atomic van der Waals volumes)
5	RDF s30 (unweighted)	80	RDF s105 (atomic van der Waals volumes)
6	RDF s35 (unweighted)	81	RDF s110 (atomic van der Waals volumes)
7	RDF s40 (unweighted)	82	RDF s115 (atomic van der Waals volumes)
8	RDF s45 (unweighted)	83	RDF s120 (atomic van der Waals volumes)
9	RDF s50 (unweighted)	84	RDF s125 (atomic van der Waals volumes)
10	RDF s55 (unweighted)	85	RDF s130 (atomic van der Waals volumes)
11	RDF s60 (unweighted)	86	RDF s135 (atomic van der Waals volumes)
12	RDF s65 (unweighted)	87	RDF s140 (atomic van der Waals volumes)
13	RDF s70 (unweighted)	88	RDF s145 (atomic van der Waals volumes)



2.5.13. Molecular descriptors : RDF descriptors

14	RDF s75 (unweighted)	89	RDF s150 (atomic van der Waals volumes)
15	RDF s80 (unweighted)	90	RDF s155 (atomic van der Waals volumes)
16	RDF s85 (unweighted)	91	RDF s10 (atomic Sanderson electronegativities)
17	RDF s90 (unweighted)	92	RDF s15 (atomic Sanderson electronegativities)
18	RDF s95 (unweighted)	93	RDF s20 (atomic Sanderson electronegativities)
19	RDF s100 (unweighted)	94	RDF s25 (atomic Sanderson electronegativities)
20	RDF s105 (unweighted)	95	RDF s30 (atomic Sanderson electronegativities)
21	RDF s110 (unweighted)	96	RDF s35 (atomic Sanderson electronegativities)
22	RDF s115 (unweighted)	97	RDF s40 (atomic Sanderson electronegativities)
23	RDF s120 (unweighted)	98	RDF s45 (atomic Sanderson electronegativities)
24	RDF s125 (unweighted)	99	RDF s50 (atomic Sanderson electronegativities)
25	RDF s130 (unweighted)	100	RDF s55 (atomic Sanderson electronegativities)
26	RDF s135 (unweighted)	101	RDF s60 (atomic Sanderson electronegativities)
27	RDF s140 (unweighted)	102	RDF s65 (atomic Sanderson electronegativities)
28	RDF s145 (unweighted)	103	RDF s70 (atomic Sanderson electronegativities)
29	RDF s150 (unweighted)	104	RDF s75 (atomic Sanderson electronegativities)
30	RDF s155 (unweighted)	105	RDF s80 (atomic Sanderson electronegativities)
31	RDF s10 (atomic masses)	106	RDF s85 (atomic Sanderson electronegativities)
32	RDF s15 (atomic masses)	107	RDF s90 (atomic Sanderson electronegativities)
33	RDF s20 (atomic masses)	108	RDF s95 (atomic Sanderson electronegativities)
34	RDF s25 (atomic masses)	109	RDF s100 (atomic Sanderson electronegativities)
35	RDF s30 (atomic masses)	110	RDF s105 (atomic Sanderson electronegativities)
36	RDF s35 (atomic masses)	111	RDF s110 (atomic Sanderson electronegativities)
37	RDF s40 (atomic masses)	112	RDF s115 (atomic Sanderson electronegativities)
38	RDF s45 (atomic masses)	113	RDF s120 (atomic Sanderson electronegativities)



2.5.13. Molecular descriptors : RDF descriptors

39	RDF s50 (atomic masses)	114	RDF s125 (atomic Sanderson electronegativities)
40	RDF s55 (atomic masses)	115	RDF s130 (atomic Sanderson electronegativities)
41	RDF s60 (atomic masses)	116	RDF s135 (atomic Sanderson electronegativities)
42	RDF s65 (atomic masses)	117	RDF s140 (atomic Sanderson electronegativities)
43	RDF s70 (atomic masses)	118	RDF s145 (atomic Sanderson electronegativities)
44	RDF s75 (atomic masses)	119	RDF s150 (atomic Sanderson electronegativities)
45	RDF s80 (atomic masses)	120	RDF s155 (atomic Sanderson electronegativities)
46	RDF s85 (atomic masses)	121	RDF s10 (atomic polarizabilities)
47	RDF s90 (atomic masses)	122	RDF s15 (atomic polarizabilities)
48	RDF s95 (atomic masses)	123	RDF s20 (atomic polarizabilities)
49	RDF s100 (atomic masses)	124	RDF s25 (atomic polarizabilities)
50	RDF s105 (atomic masses)	125	RDF s30 (atomic polarizabilities)
51	RDF s110 (atomic masses)	126	RDF s35 (atomic polarizabilities)
52	RDF s115 (atomic masses)	127	RDF s40 (atomic polarizabilities)
53	RDF s120 (atomic masses)	128	RDF s45 (atomic polarizabilities)
54	RDF s125 (atomic masses)	129	RDF s50 (atomic polarizabilities)
55	RDF s130 (atomic masses)	130	RDF s55 (atomic polarizabilities)
56	RDF s135 (atomic masses)	131	RDF s60 (atomic polarizabilities)
57	RDF s140 (atomic masses)	132	RDF s65 (atomic polarizabilities)
58	RDF s145 (atomic masses)	133	RDF s70 (atomic polarizabilities)
59	RDF s150 (atomic masses)	134	RDF s75 (atomic polarizabilities)
60	RDF s155 (atomic masses)	135	RDF s80 (atomic polarizabilities)
61	RDF s10 (atomic van der Waals volumes)	136	RDF s85 (atomic polarizabilities)
62	RDF s15 (atomic van der Waals volumes)	137	RDF s90 (atomic polarizabilities)
63	RDF s20 (atomic van der Waals volumes)	138	RDF s95 (atomic polarizabilities)



2.5.13. Molecular descriptors : RDF descriptors

64	RDF s25 (atomic van der Waals volumes)	139	RDF s100 (atomic polarizabilities)
65	RDF s30 (atomic van der Waals volumes)	140	RDF s105 (atomic polarizabilities)
66	RDF s35 (atomic van der Waals volumes)	141	RDF s110 (atomic polarizabilities)
67	RDF s40 (atomic van der Waals volumes)	142	RDF s115 (atomic polarizabilities)
68	RDF s45 (atomic van der Waals volumes)	143	RDF s120 (atomic polarizabilities)
69	RDF s50 (atomic van der Waals volumes)	144	RDF s125 (atomic polarizabilities)
70	RDF s55 (atomic van der Waals volumes)	145	RDF s130 (atomic polarizabilities)
71	RDF s60 (atomic van der Waals volumes)	146	RDF s135 (atomic polarizabilities)
72	RDF s65 (atomic van der Waals volumes)	147	RDF s140 (atomic polarizabilities)
73	RDF s70 (atomic van der Waals volumes)	148	RDF s145 (atomic polarizabilities)
74	RDF s75 (atomic van der Waals volumes)	149	RDF s150 (atomic polarizabilities)
75	RDF s80 (atomic van der Waals volumes)	150	RDF s155 (atomic polarizabilities)

2.5.14. Molecular descriptors : 3D-MoRSE descriptors

1	3D-MoRSE s1 (unweighted)	81	3D-MoRSE s17 (atomic van der Waals volumes)
2	3D-MoRSE s2 (unweighted)	82	3D-MoRSE s18 (atomic van der Waals volumes)
3	3D-MoRSE s3 (unweighted)	83	3D-MoRSE s19 (atomic van der Waals volumes)
4	3D-MoRSE s4 (unweighted)	84	3D-MoRSE s20 (atomic van der Waals volumes)
5	3D-MoRSE s5 (unweighted)	85	3D-MoRSE s21 (atomic van der Waals volumes)
6	3D-MoRSE s6 (unweighted)	86	3D-MoRSE s22 (atomic van der Waals volumes)
7	3D-MoRSE s7 (unweighted)	87	3D-MoRSE s23 (atomic van der Waals volumes)
8	3D-MoRSE s8 (unweighted)	88	3D-MoRSE s24 (atomic van der Waals volumes)
9	3D-MoRSE s9 (unweighted)	89	3D-MoRSE s25 (atomic van der Waals volumes)
10	3D-MoRSE s10 (unweighted)	90	3D-MoRSE s26 (atomic van der Waals volumes)



2.5.14. Molecular descriptors : 3D-MoRSE descriptors

11	3D-MoRSE s11 (unweighted)	91	3D-MoRSE s27 (atomic van der Waals volumes)
12	3D-MoRSE s12 (unweighted)	92	3D-MoRSE s28 (atomic van der Waals volumes)
13	3D-MoRSE s13 (unweighted)	93	3D-MoRSE s29 (atomic van der Waals volumes)
14	3D-MoRSE s14 (unweighted)	94	3D-MoRSE s30 (atomic van der Waals volumes)
15	3D-MoRSE s15 (unweighted)	95	3D-MoRSE s31 (atomic van der Waals volumes)
16	3D-MoRSE s16 (unweighted)	96	3D-MoRSE s32 (atomic van der Waals volumes)
17	3D-MoRSE s17 (unweighted)	97	3D-MoRSE s1 (atomic Sanderson electronegativities)
18	3D-MoRSE s18 (unweighted)	98	3D-MoRSE s2 (atomic Sanderson electronegativities)
19	3D-MoRSE s19 (unweighted)	99	3D-MoRSE s3 (atomic Sanderson electronegativities)
20	3D-MoRSE s20 (unweighted)	100	3D-MoRSE s4 (atomic Sanderson electronegativities)
21	3D-MoRSE s21 (unweighted)	101	3D-MoRSE s5 (atomic Sanderson electronegativities)
22	3D-MoRSE s22 (unweighted)	102	3D-MoRSE s6 (atomic Sanderson electronegativities)
23	3D-MoRSE s23 (unweighted)	103	3D-MoRSE s7 (atomic Sanderson electronegativities)
24	3D-MoRSE s24 (unweighted)	104	3D-MoRSE s8 (atomic Sanderson electronegativities)
25	3D-MoRSE s25 (unweighted)	105	3D-MoRSE s9 (atomic Sanderson electronegativities)
26	3D-MoRSE s26 (unweighted)	106	3D-MoRSE s10 (atomic Sanderson electronegativities)
27	3D-MoRSE s27 (unweighted)	107	3D-MoRSE s11 (atomic Sanderson electronegativities)
28	3D-MoRSE s28 (unweighted)	108	3D-MoRSE s12 (atomic Sanderson electronegativities)
29	3D-MoRSE s29 (unweighted)	109	3D-MoRSE s13 (atomic Sanderson electronegativities)
30	3D-MoRSE s30 (unweighted)	110	3D-MoRSE s14 (atomic Sanderson electronegativities)
31	3D-MoRSE s31 (unweighted)	111	3D-MoRSE s15 (atomic Sanderson electronegativities)
32	3D-MoRSE s32 (unweighted)	112	3D-MoRSE s16 (atomic Sanderson electronegativities)
33	3D-MoRSE s1 (atomic masses)	113	3D-MoRSE s17 (atomic Sanderson electronegativities)
34	3D-MoRSE s2 (atomic masses)	114	3D-MoRSE s18 (atomic Sanderson electronegativities)
35	3D-MoRSE s3 (atomic masses)	115	3D-MoRSE s19 (atomic Sanderson electronegativities)



2.5.14. Molecular descriptors : 3D-MoRSE descriptors

36	3D-MoRSE s4 (atomic masses)	116	3D-MoRSE s20 (atomic Sanderson electronegativities)
37	3D-MoRSE s5 (atomic masses)	117	3D-MoRSE s21 (atomic Sanderson electronegativities)
38	3D-MoRSE s6 (atomic masses)	118	3D-MoRSE s22 (atomic Sanderson electronegativities)
39	3D-MoRSE s7 (atomic masses)	119	3D-MoRSE s23 (atomic Sanderson electronegativities)
40	3D-MoRSE s8 (atomic masses)	120	3D-MoRSE s24 (atomic Sanderson electronegativities)
41	3D-MoRSE s9 (atomic masses)	121	3D-MoRSE s25 (atomic Sanderson electronegativities)
42	3D-MoRSE s10 (atomic masses)	122	3D-MoRSE s26 (atomic Sanderson electronegativities)
43	3D-MoRSE s11 (atomic masses)	123	3D-MoRSE s27 (atomic Sanderson electronegativities)
44	3D-MoRSE s12 (atomic masses)	124	3D-MoRSE s28 (atomic Sanderson electronegativities)
45	3D-MoRSE s13 (atomic masses)	125	3D-MoRSE s29 (atomic Sanderson electronegativities)
46	3D-MoRSE s14 (atomic masses)	126	3D-MoRSE s30 (atomic Sanderson electronegativities)
47	3D-MoRSE s15 (atomic masses)	127	3D-MoRSE s31 (atomic Sanderson electronegativities)
48	3D-MoRSE s16 (atomic masses)	128	3D-MoRSE s32 (atomic Sanderson electronegativities)
49	3D-MoRSE s17 (atomic masses)	129	3D-MoRSE s1 (atomic polarizabilities)
50	3D-MoRSE s18 (atomic masses)	130	3D-MoRSE s2 (atomic polarizabilities)
51	3D-MoRSE s19 (atomic masses)	131	3D-MoRSE s3 (atomic polarizabilities)
52	3D-MoRSE s20 (atomic masses)	132	3D-MoRSE s4 (atomic polarizabilities)
53	3D-MoRSE s21 (atomic masses)	133	3D-MoRSE s5 (atomic polarizabilities)
54	3D-MoRSE s22 (atomic masses)	134	3D-MoRSE s6 (atomic polarizabilities)
55	3D-MoRSE s23 (atomic masses)	135	3D-MoRSE s7 (atomic polarizabilities)
56	3D-MoRSE s24 (atomic masses)	136	3D-MoRSE s8 (atomic polarizabilities)
57	3D-MoRSE s25 (atomic masses)	137	3D-MoRSE s9 (atomic polarizabilities)
58	3D-MoRSE s26 (atomic masses)	138	3D-MoRSE s10 (atomic polarizabilities)
59	3D-MoRSE s27 (atomic masses)	139	3D-MoRSE s11 (atomic polarizabilities)
60	3D-MoRSE s28 (atomic masses)	140	3D-MoRSE s12 (atomic polarizabilities)



2.5.14. Molecular descriptors : 3D-MoRSE descriptors

61	3D-MoRSE s29 (atomic masses)	141	3D-MoRSE s13 (atomic polarizabilities)
62	3D-MoRSE s30 (atomic masses)	142	3D-MoRSE s14 (atomic polarizabilities)
63	3D-MoRSE s31 (atomic masses)	143	3D-MoRSE s15 (atomic polarizabilities)
64	3D-MoRSE s32 (atomic masses)	144	3D-MoRSE s16 (atomic polarizabilities)
65	3D-MoRSE s1 (atomic van der Waals volumes)	145	3D-MoRSE s17 (atomic polarizabilities)
66	3D-MoRSE s2 (atomic van der Waals volumes)	146	3D-MoRSE s18 (atomic polarizabilities)
67	3D-MoRSE s3 (atomic van der Waals volumes)	147	3D-MoRSE s19 (atomic polarizabilities)
68	3D-MoRSE s4 (atomic van der Waals volumes)	148	3D-MoRSE s20 (atomic polarizabilities)
69	3D-MoRSE s5 (atomic van der Waals volumes)	149	3D-MoRSE s21 (atomic polarizabilities)
70	3D-MoRSE s6 (atomic van der Waals volumes)	150	3D-MoRSE s22 (atomic polarizabilities)
71	3D-MoRSE s7 (atomic van der Waals volumes)	151	3D-MoRSE s23 (atomic polarizabilities)
72	3D-MoRSE s8 (atomic van der Waals volumes)	152	3D-MoRSE s24 (atomic polarizabilities)
73	3D-MoRSE s9 (atomic van der Waals volumes)	153	3D-MoRSE s25 (atomic polarizabilities)
74	3D-MoRSE s10 (atomic van der Waals volumes)	154	3D-MoRSE s26 (atomic polarizabilities)
75	3D-MoRSE s11 (atomic van der Waals volumes)	155	3D-MoRSE s27 (atomic polarizabilities)
76	3D-MoRSE s12 (atomic van der Waals volumes)	156	3D-MoRSE s28 (atomic polarizabilities)
77	3D-MoRSE s13 (atomic van der Waals volumes)	157	3D-MoRSE s29 (atomic polarizabilities)
78	3D-MoRSE s14 (atomic van der Waals volumes)	158	3D-MoRSE s30 (atomic polarizabilities)
79	3D-MoRSE s15 (atomic van der Waals volumes)	159	3D-MoRSE s31 (atomic polarizabilities)
80	3D-MoRSE s16 (atomic van der Waals volumes)	160	3D-MoRSE s32 (atomic polarizabilities)

2.5.15. Molecular descriptors : WHIM descriptors

1	1st comp. directional WHIM size (unweighted)	51	2nd comp. directional WHIM symmetry (atomic polarizabilities)
2	2nd comp. directional WHIM size (unweighted)	52	3rd comp. directional WHIM symmetry (atomic polarizabilities)



2.5.15. Molecular descriptors : WHIM descriptors

3	3rd comp. directional WHIM size (unweighted)	53	1st comp. directional WHIM accessibility (atomic polarizabilities)
4	1st comp. directional WHIM shape (unweighted)	54	2nd comp. directional WHIM accessibility (atomic polarizabilities)
5	2nd comp. directional WHIM shape (unweighted)	55	3rd comp. directional WHIM accessibility (atomic polarizabilities)
6	1st comp. directional WHIM symmetry (unweighted)	56	1st comp. directional WHIM size (atomic electro-topological states)
7	2nd comp. directional WHIM symmetry (unweighted)	57	2nd comp. directional WHIM size (atomic electro-topological states)
8	3rd comp. directional WHIM symmetry (unweighted)	58	3rd comp. directional WHIM size (atomic electro-topological states)
9	1st comp. directional WHIM accessibility (unweighted)	59	1st comp. directional WHIM shape (atomic electro-topological states)
10	2nd comp. directional WHIM accessibility (unweighted)	60	2nd comp. directional WHIM shape (atomic electro-topological states)
11	3rd comp. directional WHIM accessibility (unweighted)	61	1st comp. directional WHIM symmetry (atomic electro-topological states)
12	1st comp. directional WHIM size (atomic masses)	62	2nd comp. directional WHIM symmetry (atomic electro-topological states)
13	2nd comp. directional WHIM size (atomic masses)	63	3rd comp. directional WHIM symmetry (atomic electro-topological states)
14	3rd comp. directional WHIM size (atomic masses)	64	1st comp. directional WHIM accessibility (atomic electro-topological states)
15	1st comp. directional WHIM shape (atomic masses)	65	2nd comp. directional WHIM accessibility (atomic electro-topological states)
16	2nd comp. directional WHIM shape (atomic masses)	66	3rd comp. directional WHIM accessibility (atomic electro-topological states)
17	1st comp. directional WHIM symmetry (atomic masses)	67	WHIM total size T (unweighted)
18	2nd comp. directional WHIM symmetry (atomic masses)	68	WHIM total size T (atomic masses)
19	3rd comp. directional WHIM symmetry (atomic masses)	69	WHIM total size T (atomic van der Waals volumes)
20	1st comp. directional WHIM accessibility (atomic masses)	70	WHIM total size T (atomic Sanderson electronegativities)
21	2nd comp. directional WHIM accessibility (atomic masses)	71	WHIM total size T (atomic polarizabilities)
22	3rd comp. directional WHIM accessibility (atomic masses)	72	WHIM total size T (atomic electro-topological states)
23	1st comp. directional WHIM size (atomic van der Waals volumes)	73	WHIM total size A (unweighted)
24	2nd comp. directional WHIM size (atomic van der Waals volumes)	74	WHIM total size A (atomic masses)
25	3rd comp. directional WHIM size (atomic van der Waals volumes)	75	WHIM total size A (atomic van der Waals volumes)
26	1st comp. directional WHIM shape (atomic van der Waals volumes)	76	WHIM total size A (atomic Sanderson electronegativities)
27	2nd comp. directional WHIM shape (atomic van der Waals volumes)	77	WHIM total size A (atomic polarizabilities)



2.5.15. Molecular descriptors : WHIM descriptors

28	1st comp. directional WHIM symmetry (atomic van der Waals volumes)	78	WHIM total size A (atomic electro-topological states)
29	2nd comp. directional WHIM symmetry (atomic van der Waals volumes)	79	WHIM total symmetry (unweighted)
30	3rd comp. directional WHIM symmetry (atomic van der Waals volumes)	80	WHIM total symmetry (atomic masses)
31	1st comp. directional WHIM accessibility (atomic van der Waals volumes)	81	WHIM total symmetry (atomic electro-topological states)
32	2nd comp. directional WHIM accessibility (atomic van der Waals volumes)	82	WHIM global shape (unweighted)
33	3rd comp. directional WHIM accessibility (atomic van der Waals volumes)	83	WHIM global shape (atomic masses)
34	1st comp. directional WHIM size (atomic Sanderson electronegativities)	84	WHIM global shape (atomic van der Waals volumes)
35	2nd comp. directional WHIM size (atomic Sanderson electronegativities)	85	WHIM global shape (atomic Sanderson electronegativities)
36	3rd comp. directional WHIM size (atomic Sanderson electronegativities)	86	WHIM global shape (atomic polarizabilities)
37	1st comp. directional WHIM shape (atomic Sanderson electronegativities)	87	WHIM global shape (atomic electro-topological states)
38	2nd comp. directional WHIM shape (atomic Sanderson electronegativities)	88	WHIM total accessibility (unweighted)
39	1st comp. directional WHIM symmetry (atomic Sanderson electronegativities)	89	WHIM total accessibility (atomic masses)
40	2nd comp. directional WHIM symmetry (atomic Sanderson electronegativities)	90	WHIM total accessibility (atomic van der Waals volumes)
41	3rd comp. directional WHIM symmetry (atomic Sanderson electronegativities)	91	WHIM total accessibility (atomic Sanderson electronegativities)
42	1st comp. directional WHIM accessibility (atomic Sanderson electronegativities)	92	WHIM total accessibility (atomic polarizabilities)
43	2nd comp. directional WHIM accessibility (atomic Sanderson electronegativities)	93	WHIM total accessibility (atomic electro-topological states)
44	3rd comp. directional WHIM accessibility (atomic Sanderson electronegativities)	94	WHIM total size V (unweighted)
45	1st comp. directional WHIM size (atomic polarizabilities)	95	WHIM total size V (atomic masses)
46	2nd comp. directional WHIM size (atomic polarizabilities)	96	WHIM total size V (atomic van der Waals volumes)
47	3rd comp. directional WHIM size (atomic polarizabilities)	97	WHIM total size V (atomic Sanderson electronegativities)
48	1st comp. directional WHIM shape (atomic polarizabilities)	98	WHIM total size V (atomic polarizabilities)
49	2nd comp. directional WHIM shape (atomic polarizabilities)	99	WHIM total size V (atomic electro-topological states)
50	1st comp. directional WHIM symmetry (atomic polarizabilities)		



2.5.16. Molecular descriptors : GETAWAY descriptors

1	GETAWAY total information content	100	GETAWAY HATS k5 (atomic polarizabilities)
2	GETAWAY standardized information content	101	GETAWAY HATS k6 (atomic polarizabilities)
3	GETAWAY mean information content	102	GETAWAY HATS k7 (atomic polarizabilities)
4	GETAWAY geometric mean	103	GETAWAY HATS k8 (atomic polarizabilities)
5	GETAWAY H k0 (unweighted)	104	GETAWAY HATS total (atomic polarizabilities)
6	GETAWAY H k1 (unweighted)	105	GETAWAY R matrix connectivity
7	GETAWAY H k2 (unweighted)	106	GETAWAY R matrix avg row sum
8	GETAWAY H k3 (unweighted)	107	GETAWAY R matrix 1st eigenvalue
9	GETAWAY H k4 (unweighted)	108	GETAWAY R k1 (unweighted)
10	GETAWAY H k5 (unweighted)	109	GETAWAY R k2 (unweighted)
11	GETAWAY H k6 (unweighted)	110	GETAWAY R k3 (unweighted)
12	GETAWAY H k7 (unweighted)	111	GETAWAY R k4 (unweighted)
13	GETAWAY H k8 (unweighted)	112	GETAWAY R k5 (unweighted)
14	GETAWAY H total (unweighted)	113	GETAWAY R k6 (unweighted)
15	GETAWAY HATS k0 (unweighted)	114	GETAWAY R k7 (unweighted)
16	GETAWAY HATS k1 (unweighted)	115	GETAWAY R k8 (unweighted)
17	GETAWAY HATS k2 (unweighted)	116	GETAWAY R total (unweighted)
18	GETAWAY HATS k3 (unweighted)	117	GETAWAY R max k1 (unweighted)
19	GETAWAY HATS k4 (unweighted)	118	GETAWAY R max k2 (unweighted)
20	GETAWAY HATS k5 (unweighted)	119	GETAWAY R max k3 (unweighted)
21	GETAWAY HATS k6 (unweighted)	120	GETAWAY R max k4 (unweighted)
22	GETAWAY HATS k7 (unweighted)	121	GETAWAY R max k5 (unweighted)
23	GETAWAY HATS k8 (unweighted)	122	GETAWAY R max k6 (unweighted)
24	GETAWAY HATS total (unweighted)	123	GETAWAY R max k7 (unweighted)



2.5.16. Molecular descriptors : GETAWAY descriptors

25	GETAWAY H k0 (atomic masses)	124	GETAWAY R max k8 (unweighted)
26	GETAWAY H k1 (atomic masses)	125	GETAWAY R max (unweighted)
27	GETAWAY H k2 (atomic masses)	126	GETAWAY R k1 (atomic masses)
28	GETAWAY H k3 (atomic masses)	127	GETAWAY R k2 (atomic masses)
29	GETAWAY H k4 (atomic masses)	128	GETAWAY R k3 (atomic masses)
30	GETAWAY H k5 (atomic masses)	129	GETAWAY R k4 (atomic masses)
31	GETAWAY H k6 (atomic masses)	130	GETAWAY R k5 (atomic masses)
32	GETAWAY H k7 (atomic masses)	131	GETAWAY R k6 (atomic masses)
33	GETAWAY H k8 (atomic masses)	132	GETAWAY R k7 (atomic masses)
34	GETAWAY H total (atomic masses)	133	GETAWAY R k8 (atomic masses)
35	GETAWAY HATS k0 (atomic masses)	134	GETAWAY R total (atomic masses)
36	GETAWAY HATS k1 (atomic masses)	135	GETAWAY R max k1 (atomic masses)
37	GETAWAY HATS k2 (atomic masses)	136	GETAWAY R max k2 (atomic masses)
38	GETAWAY HATS k3 (atomic masses)	137	GETAWAY R max k3 (atomic masses)
39	GETAWAY HATS k4 (atomic masses)	138	GETAWAY R max k4 (atomic masses)
40	GETAWAY HATS k5 (atomic masses)	139	GETAWAY R max k5 (atomic masses)
41	GETAWAY HATS k6 (atomic masses)	140	GETAWAY R max k6 (atomic masses)
42	GETAWAY HATS k7 (atomic masses)	141	GETAWAY R max k7 (atomic masses)
43	GETAWAY HATS k8 (atomic masses)	142	GETAWAY R max k8 (atomic masses)
44	GETAWAY HATS total (atomic masses)	143	GETAWAY R max (atomic masses)
45	GETAWAY H k0 (atomic van der Waals volumes)	144	GETAWAY R k1 (atomic van der Waals volumes)
46	GETAWAY H k1 (atomic van der Waals volumes)	145	GETAWAY R k2 (atomic van der Waals volumes)
47	GETAWAY H k2 (atomic van der Waals volumes)	146	GETAWAY R k3 (atomic van der Waals volumes)
48	GETAWAY H k3 (atomic van der Waals volumes)	147	GETAWAY R k4 (atomic van der Waals volumes)
49	GETAWAY H k4 (atomic van der Waals volumes)	148	GETAWAY R k5 (atomic van der Waals volumes)



2.5.16. Molecular descriptors : GETAWAY descriptors

50	GETAWAY H k5 (atomic van der Waals volumes)	149	GETAWAY R k6 (atomic van der Waals volumes)
51	GETAWAY H k6 (atomic van der Waals volumes)	150	GETAWAY R k7 (atomic van der Waals volumes)
52	GETAWAY H k7 (atomic van der Waals volumes)	151	GETAWAY R k8 (atomic van der Waals volumes)
53	GETAWAY H k8 (atomic van der Waals volumes)	152	GETAWAY R total (atomic van der Waals volumes)
54	GETAWAY H total (atomic van der Waals volumes)	153	GETAWAY R max k1 (atomic van der Waals volumes)
55	GETAWAY HATS k0 (atomic van der Waals volumes)	154	GETAWAY R max k2 (atomic van der Waals volumes)
56	GETAWAY HATS k1 (atomic van der Waals volumes)	155	GETAWAY R max k3 (atomic van der Waals volumes)
57	GETAWAY HATS k2 (atomic van der Waals volumes)	156	GETAWAY R max k4 (atomic van der Waals volumes)
58	GETAWAY HATS k3 (atomic van der Waals volumes)	157	GETAWAY R max k5 (atomic van der Waals volumes)
59	GETAWAY HATS k4 (atomic van der Waals volumes)	158	GETAWAY R max k6 (atomic van der Waals volumes)
60	GETAWAY HATS k5 (atomic van der Waals volumes)	159	GETAWAY R max k7 (atomic van der Waals volumes)
61	GETAWAY HATS k6 (atomic van der Waals volumes)	160	GETAWAY R max k8 (atomic van der Waals volumes)
62	GETAWAY HATS k7 (atomic van der Waals volumes)	161	GETAWAY R max (atomic van der Waals volumes)
63	GETAWAY HATS k8 (atomic van der Waals volumes)	162	GETAWAY R k1 (atomic Sanderson electronegativities)
64	GETAWAY HATS total (atomic van der Waals volumes)	163	GETAWAY R k2 (atomic Sanderson electronegativities)
65	GETAWAY H k0 (atomic Sanderson electronegativities)	164	GETAWAY R k3 (atomic Sanderson electronegativities)
66	GETAWAY H k1 (atomic Sanderson electronegativities)	165	GETAWAY R k4 (atomic Sanderson electronegativities)
67	GETAWAY H k2 (atomic Sanderson electronegativities)	166	GETAWAY R k5 (atomic Sanderson electronegativities)
68	GETAWAY H k3 (atomic Sanderson electronegativities)	167	GETAWAY R k6 (atomic Sanderson electronegativities)
69	GETAWAY H k4 (atomic Sanderson electronegativities)	168	GETAWAY R k7 (atomic Sanderson electronegativities)
70	GETAWAY H k5 (atomic Sanderson electronegativities)	169	GETAWAY R k8 (atomic Sanderson electronegativities)
71	GETAWAY H k6 (atomic Sanderson electronegativities)	170	GETAWAY R total (atomic Sanderson electronegativities)
72	GETAWAY H k7 (atomic Sanderson electronegativities)	171	GETAWAY R max k1 (atomic Sanderson electronegativities)
73	GETAWAY H k8 (atomic Sanderson electronegativities)	172	GETAWAY R max k2 (atomic Sanderson electronegativities)
74	GETAWAY H total (atomic Sanderson electronegativities)	173	GETAWAY R max k3 (atomic Sanderson electronegativities)



2.5.16. Molecular descriptors : GETAWAY descriptors

75	GETAWAY HATS k0 (atomic Sanderson electronegativities)	174	GETAWAY R max k4 (atomic Sanderson electronegativities)
76	GETAWAY HATS k1 (atomic Sanderson electronegativities)	175	GETAWAY R max k5 (atomic Sanderson electronegativities)
77	GETAWAY HATS k2 (atomic Sanderson electronegativities)	176	GETAWAY R max k6 (atomic Sanderson electronegativities)
78	GETAWAY HATS k3 (atomic Sanderson electronegativities)	177	GETAWAY R max k7 (atomic Sanderson electronegativities)
79	GETAWAY HATS k4 (atomic Sanderson electronegativities)	178	GETAWAY R max k8 (atomic Sanderson electronegativities)
80	GETAWAY HATS k5 (atomic Sanderson electronegativities)	179	GETAWAY R max (atomic Sanderson electronegativities)
81	GETAWAY HATS k6 (atomic Sanderson electronegativities)	180	GETAWAY R k1 (atomic polarizabilities)
82	GETAWAY HATS k7 (atomic Sanderson electronegativities)	181	GETAWAY R k2 (atomic polarizabilities)
83	GETAWAY HATS k8 (atomic Sanderson electronegativities)	182	GETAWAY R k3 (atomic polarizabilities)
84	GETAWAY HATS total (atomic Sanderson electronegativities)	183	GETAWAY R k4 (atomic polarizabilities)
85	GETAWAY H k0 (atomic polarizabilities)	184	GETAWAY R k5 (atomic polarizabilities)
86	GETAWAY H k1 (atomic polarizabilities)	185	GETAWAY R k6 (atomic polarizabilities)
87	GETAWAY H k2 (atomic polarizabilities)	186	GETAWAY R k7 (atomic polarizabilities)
88	GETAWAY H k3 (atomic polarizabilities)	187	GETAWAY R k8 (atomic polarizabilities)
89	GETAWAY H k4 (atomic polarizabilities)	188	GETAWAY R total (atomic polarizabilities)
90	GETAWAY H k5 (atomic polarizabilities)	189	GETAWAY R max k1 (atomic polarizabilities)
91	GETAWAY H k6 (atomic polarizabilities)	190	GETAWAY R max k2 (atomic polarizabilities)
92	GETAWAY H k7 (atomic polarizabilities)	191	GETAWAY R max k3 (atomic polarizabilities)
93	GETAWAY H k8 (atomic polarizabilities)	192	GETAWAY R max k4 (atomic polarizabilities)
94	GETAWAY H total (atomic polarizabilities)	193	GETAWAY R max k5 (atomic polarizabilities)
95	GETAWAY HATS k0 (atomic polarizabilities)	194	GETAWAY R max k6 (atomic polarizabilities)
96	GETAWAY HATS k1 (atomic polarizabilities)	195	GETAWAY R max k7 (atomic polarizabilities)
97	GETAWAY HATS k2 (atomic polarizabilities)	196	GETAWAY R max k8 (atomic polarizabilities)
98	GETAWAY HATS k3 (atomic polarizabilities)	197	GETAWAY R max (atomic polarizabilities)
99	GETAWAY HATS k4 (atomic polarizabilities)		



2.5.17. Molecular descriptors : Functional group counts

1	number of terminal primary C(sp ³)	66	number of nitriles (aliphatic)
2	number of total secondary C(sp ³)	67	number of nitriles (aromatic)
3	number of total tertiary C(sp ³)	68	number of positively charged N
4	number of total quaternary C(sp ³)	69	number of quaternary N
5	number of ring secondary C(sp ³)	70	number of hydroxylamines (aliphatic)
6	number of ring tertiary C(sp ³)	71	number of hydroxylamines (aromatic)
7	number of ring quaternary C(sp ³)	72	number of N-nitroso groups (aliphatic)
8	number of aromatic C(sp ²)	73	number of N-nitroso groups (aromatic)
9	number of unsubstituted benzene C(sp ²)	74	number of nitroso groups (aliphatic)
10	number of substituted benzene C(sp ²)	75	number of nitroso groups (aromatic)
11	number of non-aromatic conjugated C(sp ²)	76	number of nitro groups (aliphatic)
12	number of terminal primary C(sp ²)	77	number of nitro groups (aromatic)
13	number of aliphatic secondary C(sp ²)	78	number of imides
14	number of aliphatic tertiary C(sp ²)	79	number of hydrazones
15	number of allenes groups	80	number of hydroxyl groups
16	number of terminal C(sp)	81	number of aromatic hydroxyls
17	number of non-terminal C(sp)	82	number of primary alcohols
18	number of cyanates (aliphatic)	83	number of secondary alcohols
19	number of cyanates (aromatic)	84	number of tertiary alcohols
20	number of isocyanates (aliphatic)	85	number of ethers (aliphatic)
21	number of isocyanates (aromatic)	86	number of ethers (aromatic)
22	number of thiocyanates (aliphatic)	87	number of anhydrides (thio-)
23	number of thiocyanates (aromatic)	88	number of water molecules
24	number of isothiocyanates (aliphatic)	89	number of thiols



2.5.17. Molecular descriptors : Functional group counts

25	number of isothiocyanates (aromatic)	90	number of thioketones
26	number of carboxylic acids (aliphatic)	91	number of sulfides
27	number of carboxylic acids (aromatic)	92	number of disulfides
28	number of esters (aliphatic)	93	number of sulfoxides
29	number of esters (aromatic)	94	number of sulfones
30	number of primary amides (aliphatic)	95	number of sulfenic (thio-) acids
31	number of primary amides (aromatic)	96	number of sulfinic (thio-/dithio-) acids
32	number of secondary amides (aliphatic)	97	number of sulfonic (thio-/dithio-) acids
33	number of secondary amides (aromatic)	98	number of sulfuric (thio-/dithio-) acids
34	number of tertiary amides (aliphatic)	99	number of sulfites (thio-/dithio-)
35	number of tertiary amides (aromatic)	100	number of sulfonates (thio-/dithio-)
36	number of (thio-) carbamates (aliphatic)	101	number of sulfates (thio-/dithio-)
37	number of (thio-) carbamates (aromatic)	102	number of sulfonamides/sulfinamides/sulfenamides (thio-/dithio-)
38	number of thioacids (aliphatic)	103	number of Aziridines
39	number of thioacids (aromatic)	104	number of Oxiranes
40	number of dithioacids (aliphatic)	105	number of Thiranes
41	number of dithioacids (aromatic)	106	number of Azetidines
42	number of thioesters (aliphatic)	107	number of Oxetanes
43	number of thioesters (aromatic)	108	number of Thioethanes
44	number of dithioesters (aliphatic)	109	number of Pyrrolidines
45	number of dithioesters (aromatic)	110	number of Oxolanes
46	number of aldehydes (aliphatic)	111	number of th-Thiophenes
47	number of aldehydes (aromatic)	112	number of Pyrroles
48	number of ketones (aliphatic)	113	number of Pyrazoles
49	number of ketones (aromatic)	114	number of Imidazoles



2.5.17. Molecular descriptors : Functional group counts

50	number of urea (-thio) derivatives	115	number of Furanes
51	number of carbonate (-thio) derivatives	116	number of Thiophenes
52	number of amidine derivatives	117	number of Oxazoles
53	number of guanidine derivatives	118	number of Isoxazoles
54	number of imines (aliphatic)	119	number of Thiazoles
55	number of imines (aromatic)	120	number of Isothiazoles
56	number of oximes (aliphatic)	121	number of Triazoles
57	number of oximes (aromatic)	122	number of Pyridines
58	number of primary amines (aliphatic)	123	number of Pyridazines
59	number of primary amines (aromatic)	124	number of Pyrimidines
60	number of secondary amines (aliphatic)	125	number of Pyrazines
61	number of secondary amines (aromatic)	126	number of 135-Triazines
62	number of tertiary amines (aliphatic)	127	number of 124-Triazines
63	number of tertiary amines (aromatic)	128	number of donor atoms for H-bonds (N and O)
64	number of N hydrazines	129	number of acceptor atoms for H-bonds (N,O,F)
65	number of N azo-derivatives	130	number of intramolecular H-bonds

2.5.18. Molecular descriptors : Atom-centred fragments

1	CH3R / CH4	41	X-C(=X)-X
2	CH2R2	42	X--CH..X
3	CHR3	43	X--CR..X
4	CR4	44	X--CX..X
5	CH3X	45	H attached to C0(sp3) no X attached to next C
6	CH2RX	46	H attached to C1(sp3) / C0(sp2)



2.5.18. Molecular descriptors : Atom-centred fragments

7	CH2X2	47	H attached to C2(sp3) / C1(sp2) / C0(sp)
8	CHR2X	48	H attached to C3(sp3) / C2(sp2) / C3(sp2) / C3(sp)
9	CHRX2	49	H attached to heteroatom
10	CHX3	50	H attached to alpha-C
11	CR3X	51	H attached to C0(sp3) with 1X attached to next C
12	CR2X2	52	H attached to C0(sp3) with 2X attached to next C
13	CRX3	53	H attached to C0(sp3) with 3X attached to next C
14	CX4	54	H attached to C0(sp3) with 4X attached to next C
15	=CH2	55	alcohol
16	=CHR	56	phenol / enol / carboxyl OH
17	=CR2	57	=O
18	=CHX	58	Al-O-Al
19	=CRX	59	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X
20	=CX2	60	O--
21	#CH	61	R-O-O-R
22	#CR / R=C=R	62	Al-NH2
23	#CX	63	Al2-NH
24	R--CH--R	64	Al3-N
25	R--CR--R	65	Ar-NH2 / X-NH2
26	R--CX--R	66	Ar-NH-Al
27	R--CH--X	67	Ar-NAI2
28	R--CR--X	68	RCO-N< / >N-X=X
29	R--CX--X	69	Ar2NH / Ar3N / Ar2N-Al / R..N..R
30	X--CH--X	70	R#N / R=N-
31	X--CR--X	71	R--N--R / R--N--X



2.5.18. Molecular descriptors : Atom-centred fragments

32	X--CX--X	72	Ar-NO ₂ / R--N(--R)--O / RO-NO
33	R--CH..X	73	Al-NO ₂
34	R--CR..X	74	Ar-N=X / X-N=X
35	R--CX..X	75	N ⁺ (positively charged)
36	Al-CH=X	76	R-SH
37	Ar-CH=X	77	R ₂ S / RS-SR
38	Al-C(=X)-Al	78	R=S
39	Ar-C(=X)-R	79	R-SO-R
40	R-C(=X)-X / R-C#X / X=C=X	80	R-SO ₂ -R

2.5.19. Molecular descriptors : Charge descriptors

1	maximum positive charge	8	relative positive charge
2	maximum negative charge	9	relative negative charge
3	total positive charge	10	submolecular polarity parameter
4	total negative charge	11	topological electronic descriptor
5	total absolute charge	12	topological electronic descriptor (bond restricted)
6	mean absolute charge	13	partial charge weighted topological electronic descriptor
7	total squared charge	14	local dipole index

2.5.20. Molecular descriptors : Molecular properties

1	unsaturation index	14	Ghose-Viswanadhan-Wendoloski antiinflammatory (covering 50%)
2	hydrophilic factor	15	Ghose-Viswanadhan-Wendoloski antidepressant (covering 80%)
3	Ghose-Crippen molar refractivity	16	Ghose-Viswanadhan-Wendoloski antidepressant (covering 50%)



2.5.20. Molecular descriptors : Molecular properties

4	fragment-based polar surface area from N,O polar coefficients)	17	Ghose-Viswanadhan-Wendoloski antipsychotic (covering 80%)
5	fragment-based polar surface area from N,O,S,P polar coefficients)	18	Ghose-Viswanadhan-Wendoloski antipsychotic (covering 50%)
6	Moriguchi octanol-water partition coefficient (MLOGP)	19	Ghose-Viswanadhan-Wendoloski antihypertensive (covering 80%)
7	Squared Moriguchi octanol-water partition coefficient (MLOGP ²)	20	Ghose-Viswanadhan-Wendoloski antihypertensive (covering 50%)
8	Ghose-Crippen octanol-water partition coefficient (ALOGP)	21	Ghose-Viswanadhan-Wendoloski hypnotic (covering 80%)
9	Squared Ghose-Crippen octanol-water partition coefficient (ALOGP ²)	22	Ghose-Viswanadhan-Wendoloski hypnotic (covering 50%)
10	Lipinski Alert index	23	Ghose-Viswanadhan-Wendoloski antineoplastic (covering 80%)
11	Ghose-Viswanadhan-Wendoloski drug-like (covering 80%)	24	Ghose-Viswanadhan-Wendoloski antineoplastic (covering 50%)
12	Ghose-Viswanadhan-Wendoloski drug-like (covering 50%)	25	Ghose-Viswanadhan-Wendoloski antiinfective (covering 80%)
13	Ghose-Viswanadhan-Wendoloski antiinflammatory (covering 80%)	26	Ghose-Viswanadhan-Wendoloski antiinfective (covering 50%)

2.5.21. Molecular descriptors : 2D binary fingerprints

1	existence of C - C at topological distance 1	51	existence of C - C at topological distance 6
2	existence of C - N at topological distance 1	52	existence of C - N at topological distance 6
3	existence of C - O at topological distance 1	53	existence of C - O at topological distance 6
4	existence of C - S at topological distance 1	54	existence of C - S at topological distance 6
5	existence of N - N at topological distance 1	55	existence of N - N at topological distance 6
6	existence of N - O at topological distance 1	56	existence of N - O at topological distance 6
7	existence of N - S at topological distance 1	57	existence of N - S at topological distance 6
8	existence of O - O at topological distance 1	58	existence of O - O at topological distance 6
9	existence of O - S at topological distance 1	59	existence of O - S at topological distance 6
10	existence of S - S at topological distance 1	60	existence of S - S at topological distance 6
11	existence of C - C at topological distance 2	61	existence of C - C at topological distance 7
12	existence of C - N at topological distance 2	62	existence of C - N at topological distance 7



2.5.21. Molecular descriptors : 2D binary fingerprints

13	existence of C - O at topological distance 2	63	existence of C - O at topological distance 7
14	existence of C - S at topological distance 2	64	existence of C - S at topological distance 7
15	existence of N - N at topological distance 2	65	existence of N - N at topological distance 7
16	existence of N - O at topological distance 2	66	existence of N - O at topological distance 7
17	existence of N - S at topological distance 2	67	existence of N - S at topological distance 7
18	existence of O - O at topological distance 2	68	existence of O - O at topological distance 7
19	existence of O - S at topological distance 2	69	existence of O - S at topological distance 7
20	existence of S - S at topological distance 2	70	existence of S - S at topological distance 7
21	existence of C - C at topological distance 3	71	existence of C - C at topological distance 8
22	existence of C - N at topological distance 3	72	existence of C - N at topological distance 8
23	existence of C - O at topological distance 3	73	existence of C - O at topological distance 8
24	existence of C - S at topological distance 3	74	existence of C - S at topological distance 8
25	existence of N - N at topological distance 3	75	existence of N - N at topological distance 8
26	existence of N - O at topological distance 3	76	existence of N - O at topological distance 8
27	existence of N - S at topological distance 3	77	existence of N - S at topological distance 8
28	existence of O - O at topological distance 3	78	existence of O - O at topological distance 8
29	existence of O - S at topological distance 3	79	existence of O - S at topological distance 8
30	existence of S - S at topological distance 3	80	existence of S - S at topological distance 8
31	existence of C - C at topological distance 4	81	existence of C - C at topological distance 9
32	existence of C - N at topological distance 4	82	existence of C - N at topological distance 9
33	existence of C - O at topological distance 4	83	existence of C - O at topological distance 9
34	existence of C - S at topological distance 4	84	existence of C - S at topological distance 9
35	existence of N - N at topological distance 4	85	existence of N - N at topological distance 9
36	existence of N - O at topological distance 4	86	existence of N - O at topological distance 9
37	existence of N - S at topological distance 4	87	existence of N - S at topological distance 9



2.5.21. Molecular descriptors : 2D binary fingerprints

38	existence of O - O at topological distance 4	88	existence of O - O at topological distance 9
39	existence of O - S at topological distance 4	89	existence of O - S at topological distance 9
40	existence of S - S at topological distance 4	90	existence of S - S at topological distance 9
41	existence of C - C at topological distance 5	91	existence of C - C at topological distance 10
42	existence of C - N at topological distance 5	92	existence of C - N at topological distance 10
43	existence of C - O at topological distance 5	93	existence of C - O at topological distance 10
44	existence of C - S at topological distance 5	94	existence of C - S at topological distance 10
45	existence of N - N at topological distance 5	95	existence of N - N at topological distance 10
46	existence of N - O at topological distance 5	96	existence of N - O at topological distance 10
47	existence of N - S at topological distance 5	97	existence of N - S at topological distance 10
48	existence of O - O at topological distance 5	98	existence of O - O at topological distance 10
49	existence of O - S at topological distance 5	99	existence of O - S at topological distance 10
50	existence of S - S at topological distance 5	100	existence of S - S at topological distance 10

2.5.22. Molecular descriptors : 2D frequency fingerprints

1	frequency of C - C at topological distance 1	51	frequency of C - C at topological distance 6
2	frequency of C - N at topological distance 1	52	frequency of C - N at topological distance 6
3	frequency of C - O at topological distance 1	53	frequency of C - O at topological distance 6
4	frequency of C - S at topological distance 1	54	frequency of C - S at topological distance 6
5	frequency of N - N at topological distance 1	55	frequency of N - N at topological distance 6
6	frequency of N - O at topological distance 1	56	frequency of N - O at topological distance 6
7	frequency of N - S at topological distance 1	57	frequency of N - S at topological distance 6
8	frequency of O - O at topological distance 1	58	frequency of O - O at topological distance 6
9	frequency of O - S at topological distance 1	59	frequency of O - S at topological distance 6



2.5.22. Molecular descriptors : 2D frequency fingerprints

10	frequency of S - S at topological distance 1	60	frequency of S - S at topological distance 6
11	frequency of C - C at topological distance 2	61	frequency of C - C at topological distance 7
12	frequency of C - N at topological distance 2	62	frequency of C - N at topological distance 7
13	frequency of C - O at topological distance 2	63	frequency of C - O at topological distance 7
14	frequency of C - S at topological distance 2	64	frequency of C - S at topological distance 7
15	frequency of N - N at topological distance 2	65	frequency of N - N at topological distance 7
16	frequency of N - O at topological distance 2	66	frequency of N - O at topological distance 7
17	frequency of N - S at topological distance 2	67	frequency of N - S at topological distance 7
18	frequency of O - O at topological distance 2	68	frequency of O - O at topological distance 7
19	frequency of O - S at topological distance 2	69	frequency of O - S at topological distance 7
20	frequency of S - S at topological distance 2	70	frequency of S - S at topological distance 7
21	frequency of C - C at topological distance 3	71	frequency of C - C at topological distance 8
22	frequency of C - N at topological distance 3	72	frequency of C - N at topological distance 8
23	frequency of C - O at topological distance 3	73	frequency of C - O at topological distance 8
24	frequency of C - S at topological distance 3	74	frequency of C - S at topological distance 8
25	frequency of N - N at topological distance 3	75	frequency of N - N at topological distance 8
26	frequency of N - O at topological distance 3	76	frequency of N - O at topological distance 8
27	frequency of N - S at topological distance 3	77	frequency of N - S at topological distance 8
28	frequency of O - O at topological distance 3	78	frequency of O - O at topological distance 8
29	frequency of O - S at topological distance 3	79	frequency of O - S at topological distance 8
30	frequency of S - S at topological distance 3	80	frequency of S - S at topological distance 8
31	frequency of C - C at topological distance 4	81	frequency of C - C at topological distance 9
32	frequency of C - N at topological distance 4	82	frequency of C - N at topological distance 9
33	frequency of C - O at topological distance 4	83	frequency of C - O at topological distance 9
34	frequency of C - S at topological distance 4	84	frequency of C - S at topological distance 9



2.5.22. Molecular descriptors : 2D frequency fingerprints

35	frequency of N - N at topological distance 4	85	frequency of N - N at topological distance 9
36	frequency of N - O at topological distance 4	86	frequency of N - O at topological distance 9
37	frequency of N - S at topological distance 4	87	frequency of N - S at topological distance 9
38	frequency of O - O at topological distance 4	88	frequency of O - O at topological distance 9
39	frequency of O - S at topological distance 4	89	frequency of O - S at topological distance 9
40	frequency of S - S at topological distance 4	90	frequency of S - S at topological distance 9
41	frequency of C - C at topological distance 5	91	frequency of C - C at topological distance 10
42	frequency of C - N at topological distance 5	92	frequency of C - N at topological distance 10
43	frequency of C - O at topological distance 5	93	frequency of C - O at topological distance 10
44	frequency of C - S at topological distance 5	94	frequency of C - S at topological distance 10
45	frequency of N - N at topological distance 5	95	frequency of N - N at topological distance 10
46	frequency of N - O at topological distance 5	96	frequency of N - O at topological distance 10
47	frequency of N - S at topological distance 5	97	frequency of N - S at topological distance 10
48	frequency of O - O at topological distance 5	98	frequency of O - O at topological distance 10
49	frequency of O - S at topological distance 5	99	frequency of O - S at topological distance 10
50	frequency of S - S at topological distance 5	100	frequency of S - S at topological distance 10

2.5.23. Molecular descriptors : Quantum-chemical descriptors

1	No. of occupied electronic levels	79	FNSA-3 [QC]
2	No. of occupied electronic levels / # of atoms	80	WPSA-3 [QC]
3	HOMO-1 energy	81	WNSA-3 [QC]
4	HOMO energy	82	RPCG (most positive charge / total positive charge) [QC]
5	LUMO energy	83	RPCS (most positive surface area * RPCG) [QC]
6	LUMO+1 energy	84	RNCG (most negative charge / total positive charge) [QC]



2.5.23. Molecular descriptors : Quantum-chemical descriptors

7	HOMO - LUMO energy gap	85	RNCS (most negative surface area * RNCG) [QC]
8	min nucleophilic reactivity index (S)	86	HDSA [QC]
9	max nucleophilic reactivity index (S)	87	HFHDSA (HDSA/TMSA) [QC]
10	avg nucleophilic reactivity index (S)	88	HASA [QC]
11	min nucleophilic reactivity index (N)	89	FHASA (HASA/TMSA) [QC]
12	max nucleophilic reactivity index (N)	90	HBSA [QC]
13	avg nucleophilic reactivity index (N)	91	FHBSA (HBSA/TMSA) [QC]
14	min nucleophilic reactivity index (C)	92	HDCA [QC]
15	max nucleophilic reactivity index (C)	93	FHDCA (HDCA/TMSA) [QC]
16	avg nucleophilic reactivity index (C)	94	HACA [QC]
17	min nucleophilic reactivity index (O)	95	FHACA (HACA/TMSA) [QC]
18	max nucleophilic reactivity index (O)	96	HBCA [QC]
19	avg nucleophilic reactivity index (O)	97	FHBCA (HBCA/TMSA) [QC]
20	min electrophilic reactivity index (S)	98	min(nHA, nHD) [QC]
21	max electrophilic reactivity index (S)	99	count of HA sites [QC]
22	avg electrophilic reactivity index (S)	100	count of HD sites [QC]
23	min electrophilic reactivity index (N)	101	HA dep. HDSA-1 [QC]
24	max electrophilic reactivity index (N)	102	HA dep. HDSA-1/TMSA [QC]
25	avg electrophilic reactivity index (N)	103	HA dep. HDSA-2 [QC]
26	min electrophilic reactivity index (C)	104	HA dep. HDSA-2/TMSA [QC]
27	max electrophilic reactivity index (C)	105	HA dep. HDSA-2/sqrt(TMSA) [QC]
28	avg electrophilic reactivity index (C)	106	HA dep. HDCA-1 [QC]
29	min electrophilic reactivity index (O)	107	HA dep. HDCA-1/TMSA [QC]
30	max electrophilic reactivity index (O)	108	HA dep. HDCA-2 [QC]
31	avg electrophilic reactivity index (O)	109	HA dep. HDCA-2/TMSA [QC]



2.5.23. Molecular descriptors : Quantum-chemical descriptors

32	min 1-electron reactivity index (S)	110	HA dep. HDCA-2/sqrt(TMSA) [QC]
33	max 1-electron reactivity index (S)	111	HASA-1 [QC]
34	avg 1-electron reactivity index (S)	112	HASA-1/TMSA [QC]
35	min 1-electron reactivity index (N)	113	HASA-2 [QC]
36	max 1-electron reactivity index (N)	114	HASA-2/TMSA [QC]
37	avg 1-electron reactivity index (N)	115	HASA-2/sqrt(TMSA) [QC]
38	min 1-electron reactivity index (C)	116	HACA-1 [QC]
39	max 1-electron reactivity index (C)	117	HACA-1/TMSA [QC]
40	avg 1-electron reactivity index (C)	118	HACA-2 [QC]
41	min 1-electron reactivity index (O)	119	HACA-2/TMSA [QC]
42	max 1-electron reactivity index (O)	120	HACA-2/sqrt(TMSA) [QC]
43	avg 1-electron reactivity index (O)	121	min AO electronic populaiton
44	max net atomic charge (S)	122	max AO electronic population
45	min net atomic charge (S)	123	max bond order (sigma-sigma)
46	max net atomic charge (N)	124	max bond order (pi-pi)
47	min net atomic charge (N)	125	max bond order (sigma-pi)
48	max net atomic charge (C)	126	min valency (S)
49	min net atomic charge (C)	127	max valency (S)
50	max net atomic charge (O)	128	avg valency (S)
51	min net atomic charge (O)	129	min (>0.1) bond order (S)
52	max net atomic charge (H)	130	max bond order (S)
53	min net atomic charge (H)	131	avg bond order (S)
54	max net atomic charge	132	min valency (N)
55	min net atomic charge	133	max valency (N)
56	total molecular dipole	134	avg valency (N)



2.5.23. Molecular descriptors : Quantum-chemical descriptors

57	total point charge comp. (molecular dipole)	135	min (>0.1) bond order (N)
58	total hybridization comp. (molecular dipole)	136	max bond order (N)
59	Image of the Onsager-Kirkwood solvation energy	137	avg bond order (N)
60	TMSA [QC]	138	min valency (C)
61	PPSA-1 [QC]	139	max valency (C)
62	PNSA-1 [QC]	140	avg valency (C)
63	DPSA-1 [QC]	141	min (>0.1) bond order (C)
64	FPSA-1 [QC]	142	max bond order (C)
65	FNSA-1 [QC]	143	avg bond order (C)
66	WPSA-1 [QC]	144	min valency (O)
67	WNSA-1 [QC]	145	max valency (O)
68	PPSA-2 [QC]	146	avg valency (O)
69	PNSA-2 [QC]	147	min (>0.1) bond order (O)
70	DPSA-2 [QC]	148	max bond order (O)
71	FPSA-2 [QC]	149	avg bond order (O)
72	FNSA-2 [QC]	150	min valency (H)
73	WPSA-2 [QC]	151	max valency (H)
74	WNSA-2 [QC]	152	avg valency (H)
75	PPSA-3 [QC]	153	min (>0.1) bond order (H)
76	PNSA-3 [QC]	154	max bond order (H)
77	DPSA-3 [QC]	155	avg bond order (H)
78	FPSA-3 [QC]		



2.5.24. Molecular descriptors : Electrostatic descriptors

1	max partial charge (S) [Zefirov]	34	DPSA-3 [Zefirov]
2	min partial charge (S) [Zefirov]	35	FPSA-3 [Zefirov]
3	max partial charge (C) [Zefirov]	36	FNSA-3 [Zefirov]
4	min partial charge (C) [Zefirov]	37	WPSA-3 [Zefirov]
5	max partial charge (N) [Zefirov]	38	WNSA-3 [Zefirov]
6	min partial charge (N) [Zefirov]	39	RPCG (most positive charge / total positive charge) [Zefirov]
7	max partial charge (O) [Zefirov]	40	RPCS (most positive surface area * RPCG) [Zefirov]
8	min partial charge (O) [Zefirov]	41	RNCG (most negative charge / total positive charge) [Zefirov]
9	max partial charge (H) [Zefirov]	42	RNCS (most negative surface area * RNCG) [Zefirov]
10	min partial charge (H) [Zefirov]	43	min(nHA, nHD) [Zefirov]
11	max partial charge	44	count of HA sites [Zefirov]
12	min partial charge	45	count of HD sites [Zefirov]
13	polarity parameter	46	HA dep. HDSA-1 [Zefirov]
14	polarity parameter/square distance	47	HA dep. HDSA-1/TMSA [Zefirov]
15	Topographic electronic index (all pairs) [Zefirov]	48	HA dep. HDSA-2 [Zefirov]
16	Topographic electronic index (all bonds) [Zefirov]	49	HA dep. HDSA-2/TMSA [Zefirov]
17	TMSA [Zefirov]	50	HA dep. HDSA-2/sqrt(TMSA) [Zefirov]
18	PPSA-1 [Zefirov]	51	HA dep. HDCA-1 [Zefirov]
19	PNSA-1 [Zefirov]	52	HA dep. HDCA-1/TMSA [Zefirov]
20	DPSA-1 [Zefirov]	53	HA dep. HDCA-2 [Zefirov]
21	FPSA-1 [Zefirov]	54	HA dep. HDCA-2/TMSA [Zefirov]
22	FNSA-1 [Zefirov]	55	HA dep. HDCA-2/sqrt(TMSA) [Zefirov]
23	WPSA-1 [Zefirov]	56	HASA-1 [Zefirov]
24	WNSA-1 [Zefirov]	57	HASA-1/TMSA [Zefirov]



2.5.24. Molecular descriptors : Electrostatic descriptors

25	PPSA-2 [Zefirov]	58	HASA-2 [Zefirov]
26	PNSA-2 [Zefirov]	59	HASA-2/TMSA [Zefirov]
27	DPSA-2 [Zefirov]	60	HASA-2/sqrt(TMSA) [Zefirov]
28	FPSA-2 [Zefirov]	61	HACA-1 [Zefirov]
29	FNSA-2 [Zefirov]	62	HACA-1/TMSA [Zefirov]
30	WPSA-2 [Zefirov]	63	HACA-2 [Zefirov]
31	WNSA-2 [Zefirov]	64	HACA-2/TMSA [Zefirov]
32	PPSA-3 [Zefirov]	65	HACA-2/sqrt(TMSA) [Zefirov]
33	PNSA-3 [Zefirov]		

2.6. Drug Properties

1	Number of atoms	9	Ghose-Crippen octanol-water partition coeff. (logP)
2	molecular weight	10	Moriguchi octanol-water partition coeff. (logP)
3	dipole moment	11	Lipinski Alert index
4	LogP (Octanol-Water Partition Coefficient)	12	Drug-likeness
5	LogS (Water Solubility)	13	Activity Score for GPCR ligands
6	number of acceptor atoms for H-bonds (N,O)	14	Activity Score for Ion Channel Modulators
7	number of donor atoms for H-bonds (N,O)	15	Activity Score for Kinase Inhibitors
8	Ghose-Crippen molar refractivity	16	Activity Score for Nuclear receptor ligands



2.7. Analytical Information (based on quantum results only)

1	Geometry	3D Structure XYZ Coordinates Transformed Coordinates
2	Measurements	Distance Angle Dihedral Angle Animation of Specific Vibration Frequency Intensity Displacement Vectors
3	Spectra	IR (Infrared) VCD (Vibrational Circular Dichroism) NMR (Nuclear Magnetic Resonance) - CNMR, HNMR, NNMR, ONMR, SNMR
4	Orbital	2D Orbitals 3D Orbitals
