MolInstincts

Technical Specification

Contents

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		**2,854,056**
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**
Hydrocarbonds				
DB #04	• Hydrocarbons	1 – 57	Compounds in DB #05 – #09 (= DB #05 + DB #06 + DB #07 + DB #08 + DB #09)	**959,269**
DB #05	► Alkane	1 – 57	Alkane (Paraffin)	**212,592**
DB #06	► Alkene	2 – 30	Alkene (Olefin)	**247,638**
DB #07	► Alkyne	2 – 28	Alkyne	**77,600**
DB #08	► Cyclo-Hydrocarbons	3 – 57	Cycloalkane(Cycloparaffins, Naphthenes), Cycloalkene(Cycloolefins), Cycloalkyene	**169,568**
DB #09	► Aromatics	4 – 57	Aromatics	**251,871**
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 + DB #35 + DB #36)	**1,510,223**
DB #11	► O-Hetero Compounds	0 – 57	O-heterocyclic, carbonyl compound, aldehyde, ketone, ketene, carbonyl hydrate, hemiacetal, acetal, enol, enolether, 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.	**219,768**

*** 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. aliphat. amine, prim. aromat. amine, sec. amine, sec. aliphat. amine, sec. mixed amine (aryl alkyl), sec. aromat. amine, tert. amine, tert. aliphat. amine, tert. mixed amine, tert. aromat. amine, carboxylic acid amidine, carboxylic acid amidrazone, nitrile, guanidine, azide, azo compound, cyanate, carbodiimide	**114,388**
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	**59,748**
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	**513,065**
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, sulfinic acid, sulfinic acid ester, sulfinic acid ester, sulfinic acid ester, sulfuric acid deriv., sulfonic acid deriv., sulfinic acid deriv.	**81,469**
DB #16	► N/S-Hetero Compounds	0 – 25	thiosemicarbazone, thiohemiaminal, thiolactam, imidothioester, thioxohetarene, thiourea, isothiourea, thiosemicarbazide, thiocyanate, isothiocyanate, thiocarbamic acid deriv.	**116,134**
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	**349,114**
DB #35	► Halogen Compounds	0 – 29	fluoride, chloride, bromide, iodide, fluoro-, chloro-, bromo- or iodo- compounds	**50,290**
DB #36	► Extra-Hetero Compounds	0 – 29	silane, silinane, silolane, silyl compound, phosphane, phosphonite, phosphonate, phosphoryl compound, arsane, arsanethione, arisonic acid, arsanyl compound	**10,086**
Fuels				
DB #18	Gasoline	5 – 12	Alkane, Cycloalkane	**105,951**

Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
DB #19	Jet-fuel	10 – 15	Alkane, Aromatics	**171,891**
DB #20	Diesel	12 – 25	Alkane, Alkene, Cycloalkane, Aromatics	**735,021**
DB #21	Bio-Diesel	12 – 19	Alkane, Alkene, Cycloalkane, Aromatics	**672,068**
Chemical Process related Compounds				
DB #22	Thermal Cracking	1 – 15	Alkane, Alkene, Alkyne, Aromatics, Hydrocarbon radicals	**491,048**
DB #23	Catalytic Cracking	1 – 40	Alkane, Alkene, Aromatics, Cycloalkane	**798,965**
DB #24	Hydro Cracking	5 – 19	Alkane, Cycloalkane, Aromatics, Hydrocarbon radicals	**768,135**
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	**1,012,022**
DB #26	Isomerization	4 – 15	Alkane, Alkene, Aromatics	**231,999**
DB #27	Catalytic Reforming	6 – 15	Alkane, Alkene, Alkyne, Cycloalkane, Aromatics	**408,199**
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	**1,349,567**
DB #29	Soot	13 – 24	Aromatics	**248,137**
DB #30	Naphtha	1 – 15	Alkane, Alkene, Alkyne, Aromatics	**273,290**
DB #31	Gas-To-Liquid (GTL, CH4 Reforming + Fischer-Tropsch)	1 – 57	Parafin, Cyclo-parafin, Olefin, Cyclo-olefin, Diene, Aormatics, Alcohol, Phenol, Aldehyde, Carboxylic acid, Ester, Ketone, Acetal, Ether, Furan	**858,442**

Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
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	**1,249,279**
DB #33	Methanol-To-Olefin (MTO) / Methanol-To-Gasoline (MTG)	1 – 57	Parafin, Olefin, Aromatics, Methanol, Dimethyl Ether, Water	**689,698**
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. aliphat. amine, prim. aromat. amine, sec. amine, sec. aliphat. amine, sec. mixed amine (aryl alkyl), sec. aromat. amine, tert. amine, tert. aliphat. amine, tert. mixed amine, tert. aromat. amine, nitrile, acyl cyanide, iminohetarene, 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, oxohetarene, 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, thioxohetarene, thiocyanate, isothiocyanate, thiocarboxylic acid, thiocarboxylic acid ester, thiolactone, thiocarboxylic acid amide, thiolactam, thiocarbonic acid deriv., thiocarbonic acid monoester, thiocarbonic acid diester, thiourea, isothiourea, 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,	**1,312,153**

Database(DB) Product Number	Category of Compounds	Carbon Range	Type of Compounds	Number of Compounds
			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	

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

2.2. Thermo-Physico-Chemical Properties (constant)

16	Refractive Index	**34**	Heat of Vaporization at 298.15K
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

2.4. Quantum Information

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

2.5.1. Molecular descriptors : Constitutional descriptors

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
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 distantce 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)

2.5.2. Molecular descriptors : Topological descriptors

14	Average Complementary Information content (order 0)	**71**	Balaban-type index (van der Waals weighted distantce 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)
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**	elctrotopological 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-likeliness 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

2.5.2. Molecular descriptors : Topological descriptors

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
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

2.5.3. Molecular descriptors : Walk and path counts

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
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

2.5.4. Molecular descriptors : Connectivity indices

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
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

2.5.5. Molecular descriptors : Information indices

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
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)

2.5.6. Molecular descriptors : List of 2D autocorrelation indices

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)
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)

2.5.6. Molecular descriptors : List of 2D autocorrelation indices

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)
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

2.5.7. Molecular descriptors : Edge adjacency indices

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
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)

2.5.7. Molecular descriptors : Edge adjacency indices

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)
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)

2.5.7. Molecular descriptors : Edge adjacency indices

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)

2.5.8. Molecular descriptors : Burden eigenvalues descriptors

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)
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 distantce 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 distantce 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 distantce 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

2.5.10. Molecular descriptors : Eigenvalue-based indices

			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)
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

2.5.11. Molecular descriptors : Randic molecular profiles

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
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)

2.5.12. Molecular descriptors : Geometrical descriptors

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)
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	spherosity 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)

2.5.13. Molecular descriptors : RDF descriptors

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)
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)

2.5.13. Molecular descriptors : RDF descriptors

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)
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)

2.5.13. Molecular descriptors : RDF descriptors

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)
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)

2.5.14. Molecular descriptors : 3D-MoRSE descriptors

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)
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)

2.5.14. Molecular descriptors : 3D-MoRSE descriptors

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)
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)

2.5.14. Molecular descriptors : 3D-MoRSE descriptors

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)
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)
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)

2.5.15. Molecular descriptors : WHIM descriptors

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)
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)

2.5.15. Molecular descriptors : WHIM descriptors

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)

2.5.16. Molecular descriptors : GETAWAY descriptors

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)
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)

2.5.16. Molecular descriptors : GETAWAY descriptors

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)
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)

2.5.16. Molecular descriptors : GETAWAY descriptors

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)
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)

2.5.16. Molecular descriptors : GETAWAY descriptors

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(sp3)	**66**	number of nitriles (aliphatic)
2	number of total secondary C(sp3)	**67**	number of nitriles (aromatic)
3	number of total tertiary C(sp3)	**68**	number of positively charged N
4	number of total quaternary C(sp3)	**69**	number of quaternary N
5	number of ring secondary C(sp3)	**70**	number of hydroxylamines (aliphatic)
6	number of ring tertiary C(sp3)	**71**	number of hydroxylamines (aromatic)
7	number of ring quaternary C(sp3)	**72**	number of N-nitroso groups (aliphatic)
8	number of aromatic C(sp2)	**73**	number of N-nitroso groups (aromatic)
9	number of unsubstituted benzene C(sp2)	**74**	number of nitroso groups (aliphatic)
10	number of substituted benzene C(sp2)	**75**	number of nitroso groups (aromatic)
11	number of non-aromatic conjugated C(sp2)	**76**	number of nitro groups (aliphatic)
12	number of terminal primary C(sp2)	**77**	number of nitro groups (aromatic)
13	number of aliphatic secondary C(sp2)	**78**	number of imides
14	number of aliphatic tertiary C(sp2)	**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)

2.5.17. Molecular descriptors : Functional group counts

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
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

2.5.17. Molecular descriptors : Functional group counts

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
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

2.5.18. Molecular descriptors : Atom-centred fragments

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)
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-NAl2

2.5.18. Molecular descriptors : Atom-centred fragments

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
32	X--CX--X	**72**	Ar-NO2 / R--N(--R)--O / RO-NO
33	R--CH..X	**73**	Al-NO2
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**	R2S / 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-SO2-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 resctricted)
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%)
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

2.5.21. Molecular descriptors : 2D binary fingerprints

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
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

2.5.21. Molecular descriptors : 2D binary fingerprints

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
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

2.5.22. Molecular descriptors : 2D frequency fingerprints

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
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

2.5.22. Molecular descriptors : 2D frequency fingerprints

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
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]

2.5.23. Molecular descriptors : Quantum-chemical descriptors

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]
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]

2.5.23. Molecular descriptors : Quantum-chemical descriptors

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]
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)

2.5.23. Molecular descriptors : Quantum-chemical descriptors

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)
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)

2.5.23. Molecular descriptors : Quantum-chemical descriptors

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	man 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]

2.5.24. Molecular descriptors : Electrostatic descriptors

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]
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