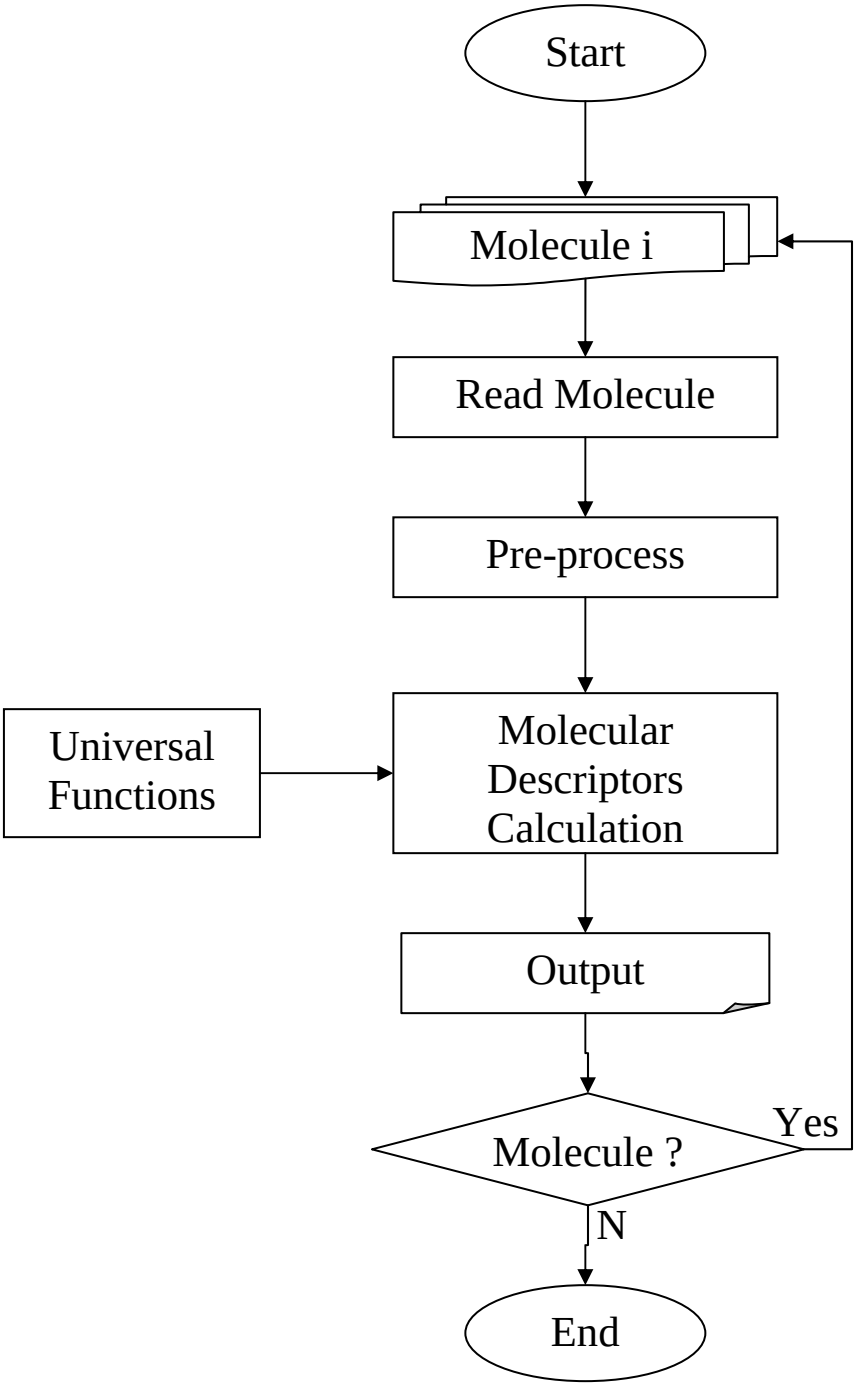
Functional Structure



Symbols and Definition

Symbole	Definition
Number	Sequence number of input structures
AUTO_ID	AUTO_ID of input structure
D001	number of 6-membered aromatic rings (only carbon atoms)
D002	Number of 03-membered rings
D003	Number of 04-membered rings
D004	Number of 05-membered rings
D005	Number of 06-membered rings
D006	Number of 07-membered rings
D007	Number of 08-membered rings
D008	Number of 09-membered rings
D009	Number of 10-membered rings
D010	Number of 11-membered rings
D011	Number of 12-membered rings
D012	number of multiple bonds
D013	number of circuits structure
D014	number of rotatable bonds
D015	rotatable bond fraction
D016	number of double bonds
D017	number of aromatic bonds
D018	sum of conventional bond orders (H-depleted)
D019	number of Hydrogen
D020	number of Helium
D021	number of Lithium
D022	number of Beryllium
D023	number of Boron
D024	number of Carbon
D025	number of Nitrogen
D026	number of Oxygen
D027	number of Fluorine
D028	number of Neon
D029	number of Sodium
D030	number of Magnesium
D031	number of Aluminum
D032	number of Silicon
D033	number of Phosphorus
D034	number of Sulfur
D035	number of Chlorine
D036	number of Argon
D037	number of Potassium
D038	number of Calcium
D039	number of Scandium
D040	number of Titanium
D041	number of Vanadium
D042	number of Chromium
D043	number of Manganese
D044	number of Iron
D045	number of Cobalt
D046	number of Nickel

D047	number of Copper
D048	number of Zinc
D049	number of Gallium
D050	number of Germanium
D051	number of Arsenic
D052	number of Selenium
D053	number of Bromine
D054	number of Krypton
D055	number of Rubidium
D056	number of Strontium
D057	number of Yttrium
D058	number of Zirconium
D059	number of Niobium
D060	number of Molybdenum
D061	number of Technetium
D062	number of Ruthenium
D063	number of Rhodium
D064	number of Palladium
D065	number of Silver
D066	number of Cadmium
D067	number of Indium
D068	number of Tin
D069	number of Antimony
D070	number of Tellurium
D071	number of Iodine
D072	number of Xenon
D073	number of Cesium
D074	number of Barium
D075	number of Lanthanum
D076	number of Cerium
D077	number of Praseodymium
D078	number of Neodymium
D079	number of Promethium
D080	number of Samarium
D081	number of Europium
D082	number of Gadolinium
D083	number of Terbium
D084	number of Dysprosium
D085	number of Holmium
D086	number of Erbium
D087	number of Thulium
D088	number of Ytterbium
D089	number of Lutetium
D090	number of Hafnium
D091	number of Tantalum
D092	number of Tungsten
D093	number of Rhenium
D094	number of Osmium
D095	number of Iridium
D096	number of Platinum

D097	number of Gold
D098	number of Mercury
D099	number of Thallium
D100	number of Lead
D101	number of Bismuth
D102	number of Polonium
D103	number of Astatine
D104	number of Radon
D105	number of Francium
D106	number of Radium
D107	number of Actinium
D108	number of Thorium
D109	number of Protactinium
D110	number of Uranium
D111	number of Neptunium
D112	number of Plutonium
D113	number of Americium
D114	number of Curium
D115	number of Berkelium
D116	number of californium
D117	number of Einsteinium
D118	number of Fermium
D119	number of Mendelevium
D120	number of Nobelium
D121	number of Lawrencium
D122	Molecular weight
D123	Average of molecular weight
D124	number of atoms in each molecule
D125	number of none-Hydrogen atoms in each molecule
D126	number of bonds in each molecule
D127	number of none-Hydrogen bonds in each molecule
D128	number of rings in each molecule
D129	number of triple bonds in each molecule
D130	number of halogen atoms in each molecule
D131	molecular size index
D132	atomic composition index
D133	mean value of atomic composition index
D134	Branch index
D135	Molecular structure connectivity index
D136	Narumi-type topological index
D137	Harmonic topological index
D138	Geometric topological index
D139	Topological distance count order-3
D140	log of vertex distance path count
D141	average of vertex distance path count
D142	Balaban type of mean square vertex distance index
D143	sum of atomic Van Der Waals Carbon-Scele
D144	mean atoic van der Waals Carbon-scale
D145	sum of atomic electronegativites Pauling-Scale on Carbon
D146	mean atomic electronegativities Pauling-scaled on Carbon

D147	sum of atomic electrongativities Sanderson-scaled on Carbon
D148	mean atomic electronegativity Sanderson-scaled on Carbon
D149	sum of atomic electrongativities Allred-Rochow-scaled on Carbon
D150	mean atomic electrongativity Allred-Rochow-scaled on Carbon
D151	sum of atomic polarizabilities scaled on Carbon-SP3
D152	mean atomic polarizability scaled on Carbon-SP3
D153	Zagreb order-1 index
D154	Zagreb order-1 index with value of valence vertex degrees
D155	Zagreb order-2 index
D156	Vertex degree topological index
D157	second Zagreb order-2 index with value of valence vertex degrees
D158	valence electrions of principal quantum index
D159	Schultz type Molecular Topological index
D160	Schultz type Molecular Topolgical Index of valence vertex degrees
D161	Molecular Topological Distance Index
D162	Molecular Topological Distance Index of valence vertex degrees
D163	Morlecular size and branching index
D164	index of terminal vertex matrix
D165	Wiener index
D166	Average Path length in Wiener Index
D167	reciprocal index of Wiener distance matrix
D168	Harary index
D169	Index of Laplacian Matrix
D170	First No-Zero eigenvalue of Laplacian matrix
D171	Wiener–Path index
D172	reciprocal Wiener-Path index
D173	Mohar order-2 index
D174	Maximum Path Index
D175	Wiener Type Maximum Path Index
D176	reciprocal Wiener Type Maximum Path Inde
D177	Minimum-Path/Maximum-Path Index
D178	All-Path Wiener - sum of the edges in the shortest paths between all pairs of non-hydrogen atoms
D179	Heteroatoms and Multiple bonds weighted Distance Matrix
D180	Mass Weighted Distance Matrix
D181	Index of Van Der Waals Weighted Distance Matrix
D182	Distance Matrix of Electronegativity Weighted with Electronegativities Pauling-Scale
D183	Distance Matrix of Electronegativity Weighted with Sanderson Electronegativities
D184	Distance Matrix of Electronegativity Weighted with Allred-Rochow Electronegativites
D185	Polarizability weighted distance matrix
D186	Average vertex distance connectivity index
D187	Balaban heteroatoms bonds weighted index
D188	Balaban mass weighted index
D189	Balaban van der Waals weighted index
D190	Balaban electronegativity weighted with Pauling-Scale index
D191	Balaban electronegativity weighted with Sanderson-Scale index
D192	Balaban electronegativity weighted with Allred-Rochow-Scale index
D193	Balaban-type polarizability weighted index
D194	maximal valence vertex electrotopological negative variation
D195	maximal valence vertex electrotopological positive variation
D196	Sum absolute electrotopological negtive variation

D197	Electrotoplogical index
D198	sum electrotopological states index
D199	mean electrotopological states index
D200	vertex connectivity order-0 index
D201	vertex connectivity order-1 index
D202	vertex connectivity order-2 index
D203	vertex connectivity order-3 index
D204	vertex connectivity order-4 index
D205	vertex connectivity order-5 index
D206	average vertex connectivity order-0 index
D207	average vertex connectivity order-1 index
D208	average vertex connectivity order-2 index
D209	average vertex connectivity order-3 index
D210	average vertex connectivity order-4 index
D211	average vertex connectivity order-5 index
D212	valence vertex connectivity order-0 Index
D213	valence vertex connectivity order-1 Index
D214	valence vertex connectivity order-2 Index
D215	valence vertex connectivity order-3 Index
D216	valence vertex connectivity order-4 Index
D217	valence vertex connectivity order-5 Index
D218	average valence vertex connectivity order-0 Index
D219	average valence vertex connectivity order-1 Index
D220	average valence vertex connectivity order-2 Index
D221	average valence vertex connectivity order-3 Index
D222	average valence vertex connectivity order-4 Index
D223	average valence vertex connectivity order-5 Index
D224	principal quantum vertex connectivity order-0 Index
D225	principal quantum vertex connectivity order-1 Index
D226	principal quantum vertex connectivity order-2 Index
D227	principal quantum vertex connectivity order-3 Index
D228	principal quantum vertex connectivity order-4 Index
D229	principal quantum vertex connectivity order-5 Index
D230	aromaticity valence vertex connectivity order-1 index
D231	sum of valence vertex connectivity order-1 index
D232	reciprocal distance order-1 sum product index
D233	squared reciprocal distance order-1 sum product index
D234	Kier atom's 0-order path information index
D235	Kier 1-path index
D236	Kier 2-path index
D237	Kier 3-path index
D238	Molecular flexibility index
D239	atom's connectivity index in longest path
D240	sum of the longest path of the atom
D241	average longest path of the molecule
D242	average of deviation of average of longest path
D243	average of deviation of distance degree
D244	shortest path in the molecule
D245	shortest path centralization index
D246	maximum value of variation

D247	EXP2 of Path-distance / Walk-distance over all atoms
D248	EXP3 of Path-distance / Walk-distance over all atoms
D249	EXP4 of Path-distance / Walk-distance over all atoms
D250	EXP5 of Path-distance / Walk-distance over all atoms
D251	Petitjean index
D252	sturcture centric index
D253	structure lopping centric group index
D254	radial centric index
D255	vertex distance count equality index
D256	vertex distance count magnitude index
D257	total vertex distance count equality index
D258	total vertex distance count magnitude index
D259	mean of distance degree equality index
D260	mean of distance degree magnitude index
D261	information of vertex degree equality index
D262	information of bonds index
D263	vertex distance path count index
D264	complexity vertex distance path count index
D265	Vertex distance information index
D266	relative of vertex distance information index
D267	mean of vertex distance information index
D268	extended of vertex distance information index
D269	information content order-0 index
D270	information content order-1 index
D271	information content order-2 index
D272	information content order-3 index
D273	information content order-4 index
D274	information content order-5 index
D275	total information content order-0 index
D276	total information content order-1 index
D277	total information content order-2 index
D278	total information content order-3 index
D279	total information content order-4 index
D280	total information content order-5 index
D281	structural information content order-0 index
D282	structural information content order-1 index
D283	structural information content order-2 index
D284	structural information content order3 index
D285	structural information content order-4 index
D286	structural information content order-5 index
D287	Complementary information content order-0 index
D288	Complementary information content order-1 index
D289	Complementary information content order-2 index
D290	Complementary information content order3 index
D291	Complementary information content order-4 index
D292	Complementary information content order-5 index
D293	bond information content order-0 index
D294	bond information content order-1 index
D295	bond information content order-2 index
D296	bond information content order3 index

D297	bond information content order-4 index
D298	bond information content order-5 index
D299	The largest eigenvalue
D300	spanning tree with log value
D301	Maximum eigenvalue weighted by Heteroatoms and Multiple bonds Matrix
D302	Maximum eigenvalue weighted by mass distance matrix
D303	Maximum eigenvalue weighted by van der Waals distance matrix
D304	Maximum eigenvalue weighted by polarizability distance matrix
D305	Maximum eigenvalue weighted by electronegativity Pauling-Scale distance matrix
D306	Maximum eigenvalue weighted by electronegativity Sanderson-Scale weighted distance matrix
D307	Maximum eigenvalue weighted by electronegativity Allred-Rochow-Scale distance matrix
D308	Sum eigenvalue weighted by Heteroatoms and Multiple bonds Distance Matrix
D309	Sum eigenvalue weighted by mass distance matrix
D310	Sum eigenvalue weighted by van der Waals distance matrix
D311	Sum eigenvalue weighted by polarizability distance matrix
D312	Sum eigenvalue weighted by electronegativity Pauling-Scale distance matrix
D313	Sum eigenvalue weighted by electronegativity Sanderson-Scale distance matrix
D314	Sum eigenvalue weighted by electronegativity Allred-Rochow-Scale distance matrix
D315	Sum absolute eigenvalue weighted by Heteroatoms and Multiple bonds Distance Matrix
D316	Sum absolute eigenvalue weighted by mass distance matrix
D317	Sum absolute eigenvalue weighted by van der Waals distance matrix
D318	Sum absolute eigenvalue weighted by polarizability distance matrix
D319	Sum absolute eigenvalue weighted by electronegativity Pauling-Scale distance matrix
D320	Sum absolute eigenvalue weighted by electronegativity Sanderson-Scale distance matrix
D321	Sum absolute eigenvalue weighted by electronegativity Allred-Rochow-Scale distance matrix
D322	distance+detour path with ring index of order 3
D323	distance+detour path with ring index of order 4
D324	distance+detour path with ring index of order 5
D325	distance+detour path with ring index of order 6
D326	distance+detour path with ring index of order 7
D327	distance+detour path with ring index of order 8
D328	distance+detour path with ring index of order 9
D329	distance+detour path with ring index of order 10
D330	distance+detour path with ring index of order 11
D331	distance+detour path with ring index of order 12
D332	distance+detour path on ring index of order 3 (circuits)
D333	distance+detour path on ring index of order 4 (circuits)
D334	distance+detour path on ring index of order 5 (circuits)
D335	distance+detour path on ring index of order 6 (circuits)
D336	distance+detour path on ring index of order 7 (circuits)
D337	distance+detour path on ring index of order 8 (circuits)
D338	distance+detour path on ring index of order 9 (circuits)
D339	distance+detour path on ring index of order 10 (circuits)
D340	distance+detour path on ring index of order 11 (circuits)
D341	distance+detour path on ring index of order 12 (circuits)
D342	molecular topological path index of order 02
D343	molecular topological path index of order 03
D344	molecular topological path index of order 04
D345	molecular topological path index of order 05
D346	molecular topological path index of order 06

D347	molecular topological path index of order 07
D348	molecular topological path index of order 08
D349	molecular topological path index of order 09
D350	molecular topological path index of order 10
D351	molecular topological multiple path index of order 03
D352	molecular topological multiple path index of order 04
D353	molecular topological multiple path index of order 05
D354	molecular topological multiple path index of order 06
D355	molecular topological multiple path index of order 07
D356	molecular topological multiple path index of order 08
D357	molecular topological multiple path index of order 09
D358	molecular topological multiple path index of order 10
D359	molecular topological all path index
D360	conventional bond index
D361	ratio of convention bonds with total path counts
D362	ratio of difference of conventional bonds and total path counts
D363	Randic index
D364	Balaban All-Path index
D365	Balaban Short-Path index
D366	sum of topological distance between the vertices N and N
D367	sum of topological distance between the vertices N and P
D368	sum of topological distance between the vertices N and O
D369	sum of topological distance between the vertices N and S
D370	sum of topological distance between the vertices N and F
D371	sum of topological distance between the vertices N and Cl
D372	sum of topological distance between the vertices N and Br
D373	sum of topological distance between the vertices N and I
D374	sum of topological distance between the vertices O and O
D375	sum of topological distance between the vertices O and S
D376	sum of topological distance between the vertices O and P
D377	sum of topological distance between the vertices O and F
D378	sum of topological distance between the vertices O and Cl
D379	sum of topological distance between the vertices O and Br
D380	sum of topological distance between the vertices O and I
D381	sum of topological distance between the vertices S and S
D382	sum of topological distance between the vertices S and P
D383	sum of topological distance between the vertices S and F
D384	sum of topological distance between the vertices S and Cl
D385	sum of topological distance between the vertices S and Br
D386	sum of topological distance between the vertices S and I
D387	sum of topological distance between the vertices P and P
D388	sum of topological distance between the vertices P and F
D389	sum of topological distance between the vertices P and Cl
D390	sum of topological distance between the vertices P and Br
D391	sum of topological distance between the vertices P and I
D392	sum of topological distance between the vertices F and F
D393	sum of topological distance between the vertices F and Cl
D394	sum of topological distance between the vertices F and Br
D395	sum of topological distance between the vertices F and I
D396	sum of topological distance between the vertices Cl and Cl

D397 sum of topological distance between the vertices Cl and Br
D398 sum of topological distance between the vertices Cl and I
D399 sum of topological distance between the vertices Br and Br
D400 sum of topological distance between the vertices Br and I
D401 sum of topological distance between the vertices I and I
D402 walk count order-01
D403 walk count order-02
D404 walk count order-03
D405 walk count order-04
D406 walk count order-05
D407 walk count order-06
D408 walk count max-10 steps
D409 walk-returning count order-1
D410 walk-returning count order-2
D411 walk-returning count order-3
D412 walk-returning count order-4
D413 walk-returning count order-5
D414 walk-returning count order-6
D415 topological structure autocorrelation length-1 weighted by atomic masses
D416 topological structure autocorrelation length-2 weighted by atomic masses
D417 topological structure autocorrelation length-3 weighted by atomic masses
D418 topological structure autocorrelation length-4 weighted by atomic masses
D419 topological structure autocorrelation length-5 weighted by atomic masses
D420 topological structure autocorrelation length-6 weighted by atomic masses
D421 topological structure autocorrelation length-7 weighted by atomic masses
D422 topological structure autocorrelation length-8 weighted by atomic masses
D423 topological structure autocorrelation length-1 weighted by atomic van der Waals volumes
D424 topological structure autocorrelation length-2 weighted by atomic van der Waals volumes
D425 topological structure autocorrelation length-3 weighted by atomic van der Waals volumes
D426 topological structure autocorrelation length-4 weighted by atomic van der Waals volumes
D427 topological structure autocorrelation length-5 weighted by atomic van der Waals volumes
D428 topological structure autocorrelation length-6 weighted by atomic van der Waals volumes
D429 topological structure autocorrelation length-7 weighted by atomic van der Waals volumes
D430 topological structure autocorrelation length-8 weighted by atomic van der Waals volumes
D431 topological structure autocorrelation length-1 weighted by atomic Sanderson electronegativities
D432 topological structure autocorrelation length-2 weighted by atomic Sanderson electronegativities
D433 topological structure autocorrelation length-3 weighted by atomic Sanderson electronegativities
D434 topological structure autocorrelation length-4 weighted by atomic Sanderson electronegativities
D435 topological structure autocorrelation length-5 weighted by atomic Sanderson electronegativities
D436 topological structure autocorrelation length-6 weighted by atomic Sanderson electronegativities
D437 topological structure autocorrelation length-7 weighted by atomic Sanderson electronegativities
D438 topological structure autocorrelation length-8 weighted by atomic Sanderson electronegativities
D439 topological structure autocorrelation length-1 weighted by atomic polarizabilities
D440 topological structure autocorrelation length-2 weighted by atomic polarizabilities
D441 topological structure autocorrelation length-3 weighted by atomic polarizabilities
D442 topological structure autocorrelation length-4 weighted by atomic polarizabilities
D443 topological structure autocorrelation length-5 weighted by atomic polarizabilities
D444 topological structure autocorrelation length-6 weighted by atomic polarizabilities
D445 topological structure autocorrelation length-7 weighted by atomic polarizabilities
D446 topological structure autocorrelation length-8 weighted by atomic polarizabilities

D447	Geary topological structure autocorrelation length-1 weighted by atomic masses
D448	Geary topological structure autocorrelation length-2 weighted by atomic masses
D449	Geary topological structure autocorrelation length-3 weighted by atomic masses
D450	Geary topological structure autocorrelation length-4 weighted by atomic masses
D451	Geary topological structure autocorrelation length-5 weighted by atomic masses
D452	Geary topological structure autocorrelation length-6 weighted by atomic masses
D453	Geary topological structure autocorrelation length-7 weighted by atomic masses
D454	Geary topological structure autocorrelation length-8 weighted by atomic masses
D455	Geary topological structure autocorrelation length-1 weighted by atomic van der Waals volumes
D456	Geary topological structure autocorrelation length-2 weighted by atomic van der Waals volumes
D457	Geary topological structure autocorrelation length-3 weighted by atomic van der Waals volumes
D458	Geary topological structure autocorrelation length-4 weighted by atomic van der Waals volumes
D459	Geary topological structure autocorrelation length-5 weighted by atomic van der Waals volumes
D460	Geary topological structure autocorrelation length-6 weighted by atomic van der Waals volumes
D461	Geary topological structure autocorrelation length-7 weighted by atomic van der Waals volumes
D462	Geary topological structure autocorrelation length-8 weighted by atomic van der Waals volumes
D463	Geary topological structure autocorrelation length-1 weighted by atomic Sanderson electronegativities
D464	Geary topological structure autocorrelation length-2 weighted by atomic Sanderson electronegativities
D465	Geary topological structure autocorrelation length-3 weighted by atomic Sanderson electronegativities
D466	Geary topological structure autocorrelation length-4 weighted by atomic Sanderson electronegativities
D467	Geary topological structure autocorrelation length-5 weighted by atomic Sanderson electronegativities
D468	Geary topological structure autocorrelation length-6 weighted by atomic Sanderson electronegativities
D469	Geary topological structure autocorrelation length-7 weighted by atomic Sanderson electronegativities
D470	Geary topological structure autocorrelation length-8 weighted by atomic Sanderson electronegativities
D471	Geary topological structure autocorrelation length-1 weighted by atomic polarizabilities
D472	Geary topological structure autocorrelation length-2 weighted by atomic polarizabilities
D473	Geary topological structure autocorrelation length-3 weighted by atomic polarizabilities
D474	Geary topological structure autocorrelation length-4 weighted by atomic polarizabilities
D475	Geary topological structure autocorrelation length-5 weighted by atomic polarizabilities
D476	Geary topological structure autocorrelation length-6 weighted by atomic polarizabilities
D477	Geary topological structure autocorrelation length-7 weighted by atomic polarizabilities
D478	Geary topological structure autocorrelation length-8 weighted by atomic polarizabilities
D479	Moran topological structure autocorrelation length-1 weighted by atomic masses
D480	Moran topological structure autocorrelation length-2 weighted by atomic masses
D481	Moran topological structure autocorrelation length-3 weighted by atomic masses
D482	Moran topological structure autocorrelation length-4 weighted by atomic masses
D483	Moran topological structure autocorrelation length-5 weighted by atomic masses
D484	Moran topological structure autocorrelation length-6 weighted by atomic masses
D485	Moran topological structure autocorrelation length-7 weighted by atomic masses
D486	Moran topological structure autocorrelation length-8 weighted by atomic masses
D487	Moran topological structure autocorrelation length-1 weighted by atomic van der Waals volumes
D488	Moran topological structure autocorrelation length-2 weighted by atomic van der Waals volumes
D489	Moran topological structure autocorrelation length-3 weighted by atomic van der Waals volumes
D490	Moran topological structure autocorrelation length-4 weighted by atomic van der Waals volumes

D491	Moran topological structure autocorrelation length-5 weighted by atomic van der Waals volumes
D492	Moran topological structure autocorrelation length-6 weighted by atomic van der Waals volumes
D493	Moran topological structure autocorrelation length-7 weighted by atomic van der Waals volumes
D494	Moran topological structure autocorrelation length-8 weighted by atomic van der Waals volumes
D495	Moran topological structure autocorrelation length-1 weighted by atomic Sanderson electronegativities
D496	Moran topological structure autocorrelation length-2 weighted by atomic Sanderson electronegativities
D497	Moran topological structure autocorrelation length-3 weighted by atomic Sanderson electronegativities
D498	Moran topological structure autocorrelation length-4 weighted by atomic Sanderson electronegativities
D499	Moran topological structure autocorrelation length-5 weighted by atomic Sanderson electronegativities
D500	Moran topological structure autocorrelation length-6 weighted by atomic Sanderson electronegativities
D501	Moran topological structure autocorrelation length-7 weighted by atomic Sanderson electronegativities
D502	Moran topological structure autocorrelation length-8 weighted by atomic Sanderson electronegativities
D503	Moran topological structure autocorrelation length-1 weighted by atomic polarizabilities
D504	Moran topological structure autocorrelation length-2 weighted by atomic polarizabilities
D505	Moran topological structure autocorrelation length-3 weighted by atomic polarizabilities
D506	Moran topological structure autocorrelation length-4 weighted by atomic polarizabilities
D507	Moran topological structure autocorrelation length-5 weighted by atomic polarizabilities
D508	Moran topological structure autocorrelation length-6 weighted by atomic polarizabilities
D509	Moran topological structure autocorrelation length-7 weighted by atomic polarizabilities
D510	Moran topological structure autocorrelation length-8 weighted by atomic polarizabilities
D511	Molecular topological order-1 charge index
D512	Molecular topological order-2 charge index
D513	Molecular topological order-3 charge index
D514	Molecular topological order-4 charge index
D515	Molecular topological order-5 charge index
D516	Molecular topological order-6 charge index
D517	Molecular topological order-7 charge index
D518	Molecular topological order-8 charge index
D519	Molecular topological order-9 charge index
D520	Molecular topological order-10 charge index
D521	Mean molecular topological order-1 charge index
D522	Mean molecular topological order-2 charge index
D523	Mean molecular topological order-3 charge index
D524	Mean molecular topological order-4 charge index
D525	Mean molecular topological order-5 charge index
D526	Mean molecular topological order-6 charge index
D527	Mean molecular topological order-7 charge index
D528	Mean molecular topological order-8 charge index
D529	Mean molecular topological order-9 charge index
D530	Mean molecular topological order-10 charge index
D531	Sum of molecular topological mean charge index
D532	Lowest eigenvalue from Burdex matrix weighteed by masses order-1
D533	Lowest eigenvalue from Burdex matrix weighteed by masses order-2
D534	Lowest eigenvalue from Burdex matrix weighteed by masses order-3

D535 Lowest eigenvalue from Burdex matrix weighteed by masses order-4
D536 Lowest eigenvalue from Burdex matrix weighteed by masses order-5
D537 Lowest eigenvalue from Burdex matrix weighteed by masses order-6
D538 Lowest eigenvalue from Burdex matrix weighteed by masses order-7
D539 Lowest eigenvalue from Burdex matrix weighteed by masses order-8
D540 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-1
D541 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-2
D542 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-3
D543 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-4
D544 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-5
D545 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-6
D546 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-7
D547 Lowest eigenvalue from Burdex matrix weighteed by van der Walls order-8
D548 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-1
D549 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-2
D550 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-3
D551 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-4
D552 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-5
D553 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-6
D554 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-7
D555 Lowest eigenvalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-8
D556 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-1
D557 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-2
D558 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-3
D559 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-4
D560 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-5
D561 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-6
D562 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-7
D563 Lowest eigenvalue from Burdex matrix weighteed by polarizabilities order-8
D564 Hightest eignevalue from Burdex matrix weighteed by masses order-1
D565 Hightest eignevalue from Burdex matrix weighteed by masses order-2
D566 Hightest eignevalue from Burdex matrix weighteed by masses order-3
D567 Hightest eignevalue from Burdex matrix weighteed by masses order-4
D568 Hightest eignevalue from Burdex matrix weighteed by masses order-5
D569 Hightest eignevalue from Burdex matrix weighteed by masses order-6
D570 Hightest eignevalue from Burdex matrix weighteed by masses order-7
D571 Hightest eignevalue from Burdex matrix weighteed by masses order-8
D572 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-1
D573 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-2
D574 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-3
D575 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-4
D576 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-5
D577 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-6
D578 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-7
D579 Hightest eignevalue from Burdex matrix weighteed by van der Walls order-8
D580 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-1
D581 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-2
D582 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-3
D583 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-4
D584 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-5

D585 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-6
D586 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-7
D587 Hightest eignevalue from Burdex matrix weighteed by electronegativities Sanderson-Scale order-8
D588 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-1
D589 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-2
D590 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-3
D591 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-4
D592 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-5
D593 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-6
D594 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-7
D595 Hightest eignevalue from Burdex matrix weighteed by polarizabilities order-8
D596 number of total primary C-sp3
D597 number of total secondary C-sp3
D598 number of total tertiary C-sp3
D599 number of total quaternary C-sp3
D600 number of ring secondary C-sp3
D601 number of ring tertiary C-sp3
D602 number of ring quaternary C-sp3
D603 number of unsubstituted aromatic C-sp2
D604 number of substituted aromatic C-sp2
D605 number of primary C-sp2
D606 number of secondary C-sp2
D607 number of tertiary C-sp2
D608 number of group allenes
D609 number of terminal C-sp
D610 number of non-terminal C-sp
D611 number of group cianates (aliphatic)
D612 number of group cianates (aromatic)
D613 number of group isocianates (aliphatic)
D614 number of group isocianates (aromatic)
D615 number of group thiocianates (aliphatic)
D616 number of group thiocianates (aromatic)
D617 number of group isothiocianates (aliphatic)
D618 number of group isothiocianates (aromatic)
D619 number of group carboxylic acids (aliphatic)
D620 number of group carboxylic acids (aromatic)
D621 number of group esters (aliphatic)
D622 number of group esters (aromatic)
D623 number of group primary amides (aliphatic)
D624 number of group primary amides (aromatic)
D625 number of group secondary amides (aliphatic)
D626 number of group secondary amides (aromatic)
D627 number of group tertiary amides (aliphatic)
D628 number of group tertiary amides (aromatic)
D629 number of group carbamates (aliphatic)
D630 number of group carbamates (aromatic)
D631 number of group acyl halogenides (aliphatic)
D632 number of group acyl halogenides (aromatic)
D633 number of group thioacids (aliphatic)
D634 number of group thioacids (aromatic)

D635	number of group ditioacids (aliphatic)
D636	number of group ditioacids (aromatic)
D637	number of group thioesters (aliphatic)
D638	number of group thioesters (aromatic)
D639	number of group dithioesters (aliphatic)
D640	number of group dithioesters (aromatic)
D641	number of group aldehydes (aliphatic)
D642	number of group aldehydes (aromatic)
D643	number of group ketones (aliphatic)
D644	number of group ketones (aromatic)
D645	number of group urea derivatives
D646	number of group urea derivatives (aromatic)
D647	number of group primary amines (aliphatic)
D648	number of group primary amines (aromatic)
D649	number of group secondary amines (aliphatic)
D650	number of group secondary amines (aromatic)
D651	number of group tertiary amines (aliphatic)
D652	number of group tertiary amines (aromatic)
D653	number of group N-hydrazines (aliphatic)
D654	number of group N-hydrazines (aromatic)
D655	number of group N-azo (aliphatic)
D656	number of group N-azo (aromatic)
D657	number of group nitriles (aliphatic)
D658	number of group nitriles (aromatic)
D659	number of group immines (aliphatic)
D660	number of group immines (aromatic)
D661	number of group ammonium groups (aliphatic)
D662	number of group ammonium groups (aromatic)
D663	number of group hydroxylamines (aliphatic)
D664	number of group hydroxylamines (aromatic)
D665	number of group oximes (aliphatic)
D666	number of group oximes (aromatic)
D667	number of group N-nitroso (aliphatic)
D668	number of group N-nitroso (aromatic)
D669	number of group nitroso (aliphatic)
D670	number of group nitroso (aromatic)
D671	number of group nitro (aliphatic)
D672	number of group nitro (aromatic)
D673	number of group imides
D674	number of group total hydroxyl groups
D675	number of group phenols
D676	number of group primary alcohols (aliphatic)
D677	number of group secondary alcohols (alinhatic)
D678	number of group tertiary alcohols (aliphatic)
D679	number of group ethers (aliphatic)
D680	number of group ethers (aromatic)
D681	number of group hypohalogenydes (aliphatic)
D682	number of group hypohalogenydes (aromatic)
D683	number of group water molecules
D684	number of group sulfoxides

D685	number of group sulfones
D686	number of group sulfates
D687	number of group thioles
D688	number of group thioketones
D689	number of group solfures
D690	number of group disolfures
D691	number of group sulfonic acids
D692	number of group sulfonamides
D693	number of group phosphites
D694	number of group phosphates
D695	number of group phosphothionates
D696	number of group phosphodithionates
D697	number of group phosphothioates
D698	number of group CH2X
D699	number of group CR2HX
D700	number of group CR3X
D701	number of group R=CHX
D702	number of group R=CRX
D703	number of group R#CX
D704	number of group CHRX2
D705	number of group CR2X2
D706	number of group R=CX2
D707	number of group RCX3
D708	number of group X-C on aromatic ring
D709	number of group X-C- on ring
D710	number of group X-C= on ring
D711	number of group X-C on conjugated C
D712	number of group donor atoms for H-bonds (with N and O)
D713	number of group acceptor atoms for H-bonds (N O F)
D714	number of group group CH3R and CH4
D715	number of group CH2R2
D716	number of group CHR3
D717	number of group CR4
D718	number of group CH3X
D719	number of group CH2RX
D720	number of group CH2X2
D721	number of group CHR2X
D722	number of group CHRX2
D723	number of group CHX3
D724	number of group CR3X
D725	number of group CR2X2
D726	number of group CRX3
D727	number of group CX4
D728	number of group =CH2
D729	number of group =CHR
D730	number of group =CR2
D731	number of group =CHX
D732	number of group =CRX
D733	number of group =CX2
D734	number of group #CH

D735	number of group #CR or R=C=R
D736	number of group #CX
D737	number of group R~CH~R
D738	number of group R~CR~R
D739	number of group R~CX~R
D740	number of group Al-CH=X
D741	number of group Ar-CH=X
D742	number of group Al-C(=X)-Al
D743	number of group Ar-C(=X)-R
D744	number of group R-C(=X)-X / R-C#X
D745	number of group X-C(=X)-X
D746	number of group H attached to C0(sp3) no X attached to next C
D747	number of group H attached to heteroatom
D748	number of group H attached to C0(sp3) with 1X attached to next C
D749	number of group H attached to C0(sp3) with 2X attached to next C
D750	number of group H attached to C0(sp3) with 3X attached to next C
D751	number of group H attached to C0(sp3) with 4X attached to next C
D752	number of group alcohol
D753	number of group phenol or enol or carboxyl OH
D754	number of group O=
D755	number of group Al-O-Al
D756	number of group Al-O-Ar or Ar-O-Ar or R-O-C=X
D757	number of group Al-NH2
D758	number of group Al2-NH
D759	number of group Al3-N
D760	number of group Ar-NH2 or X-NH2
D761	number of group Ar-NH-Al
D762	number of group Ar-NAl2
D763	number of group RCO-N< or >N-X=X
D764	number of group Ar2NH or Ar3N or Ar2N-Al
D765	number of group R#N or R=N-
D766	number of group Ar-NO2 or RO-NO2
D767	number of group Al-NO2
D768	number of group Ar-N=X or X-N=X
D769	number of group R-SH
D770	number of group R2S or RS-SR
D771	number of group R=S
D772	number of group R-SO-R
D773	number of group R-SO2-R
D774	unsaturation index weighted by conventional bonds order
D775	hydrophilic factor index
D776	aromatic bonds ratio
D777	Molecular regresson confficients surface LogP index