

## List of molecular descriptors calculated by Dragon

ID	Name	Description	Block
1	MW	molecular weight	Constitutional indices
2	AMW	average molecular weight	Constitutional indices
3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)	Constitutional indices
4	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)	Constitutional indices
5	Sp	sum of atomic polarizabilities (scaled on Carbon atom)	Constitutional indices
6	Si	sum of first ionization potentials (scaled on Carbon atom)	Constitutional indices
7	Mv	mean atomic van der Waals volume (scaled on Carbon atom)	Constitutional indices
8	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)	Constitutional indices
9	Mp	mean atomic polarizability (scaled on Carbon atom)	Constitutional indices
10	Mi	mean first ionization potential (scaled on Carbon atom)	Constitutional indices
11	nAT	number of atoms	Constitutional indices
12	nSK	number of non-H atoms	Constitutional indices
13	nBT	number of bonds	Constitutional indices
14	nBO	number of non-H bonds	Constitutional indices
15	nBM	number of multiple bonds	Constitutional indices
16	SCBO	sum of conventional bond orders (H-depleted)	Constitutional indices
17	RBN	number of rotatable bonds	Constitutional indices
18	RBF	rotatable bond fraction	Constitutional indices
19	nDB	number of double bonds	Constitutional indices
20	nTB	number of triple bonds	Constitutional indices
21	nAB	number of aromatic bonds	Constitutional indices
22	nH	number of Hydrogen atoms	Constitutional indices
23	nC	number of Carbon atoms	Constitutional indices
24	nN	number of Nitrogen atoms	Constitutional indices
25	nO	number of Oxygen atoms	Constitutional indices
26	nP	number of Phosphorous atoms	Constitutional indices
27	nS	number of Sulfur atoms	Constitutional indices
28	nF	number of Fluorine atoms	Constitutional indices
29	nCl	number of Chlorine atoms	Constitutional indices
30	nBR	number of Bromine atoms	Constitutional indices
31	nI	number of Iodine atoms	Constitutional indices
32	nB	number of Boron atoms	Constitutional indices
33	nHM	number of heavy atoms	Constitutional indices
34	nHet	number of heteroatoms	Constitutional indices
35	nX	number of halogen atoms	Constitutional indices
36	H%	percentage of H atoms	Constitutional indices
37	C%	percentage of C atoms	Constitutional indices
38	N%	percentage of N atoms	Constitutional indices
39	O%	percentage of O atoms	Constitutional indices
40	X%	percentage of halogen atoms	Constitutional indices
41	nCsp3	number of sp3 hybridized Carbon atoms	Constitutional indices
42	nCsp2	number of sp2 hybridized Carbon atoms	Constitutional indices
43	nCsp	number of sp hybridized Carbon atoms	Constitutional indices
44	nCIC	number of rings (cyclomatic number)	Ring descriptors
45	nCIR	number of circuits	Ring descriptors
46	TRS	total ring size	Ring descriptors
47	Rperim	ring perimeter	Ring descriptors
48	Rbrid	ring bridge count	Ring descriptors
49	MCD	molecular cyclized degree	Ring descriptors
50	RFD	ring fusion density	Ring descriptors
51	RCI	ring complexity index	Ring descriptors
52	NRS	number of ring systems	Ring descriptors
53	NNRS	normalized number of ring systems	Ring descriptors
54	nR03	number of 3-membered rings	Ring descriptors
55	nR04	number of 4-membered rings	Ring descriptors
56	nR05	number of 5-membered rings	Ring descriptors
57	nR06	number of 6-membered rings	Ring descriptors
58	nR07	number of 7-membered rings	Ring descriptors
59	nR08	number of 8-membered rings	Ring descriptors
60	nR09	number of 9-membered rings	Ring descriptors
61	nR10	number of 10-membered rings	Ring descriptors
62	nR11	number of 11-membered rings	Ring descriptors
63	nR12	number of 12-membered rings	Ring descriptors
64	nBnz	number of benzene-like rings	Ring descriptors
65	ARR	aromatic ratio	Ring descriptors
66	D/Dtr03	distance/detour ring index of order 3	Ring descriptors
67	D/Dtr04	distance/detour ring index of order 4	Ring descriptors
68	D/Dtr05	distance/detour ring index of order 5	Ring descriptors
69	D/Dtr06	distance/detour ring index of order 6	Ring descriptors
70	D/Dtr07	distance/detour ring index of order 7	Ring descriptors
71	D/Dtr08	distance/detour ring index of order 8	Ring descriptors
72	D/Dtr09	distance/detour ring index of order 9	Ring descriptors
73	D/Dtr10	distance/detour ring index of order 10	Ring descriptors
74	D/Dtr11	distance/detour ring index of order 11	Ring descriptors
75	D/Dtr12	distance/detour ring index of order 12	Ring descriptors
76	ZM1	first Zagreb index	Topological indices
77	ZM1V	first Zagreb index by valence vertex degrees	Topological indices
78	ZM1Kup	first Zagreb index by Kupchik vertex degrees	Topological indices
79	ZM1Mad	first Zagreb index by Madan vertex degrees	Topological indices
80	ZM1Per	first Zagreb index by perturbation vertex degrees	Topological indices
81	ZM1MulPer	first Zagreb index by multiplicative perturbation vertex degrees	Topological indices
82	ZM2	second Zagreb index	Topological indices
83	ZM2V	second Zagreb index by valence vertex degrees	Topological indices
84	ZM2Kup	second Zagreb index by Kupchik vertex degrees	Topological indices
85	ZM2Mad	second Zagreb index by Madan vertex degrees	Topological indices
86	ZM2Per	second Zagreb index by perturbation vertex degrees	Topological indices
87	ZM2MulPer	second Zagreb index by multiplicative perturbation vertex degrees	Topological indices
88	ON0	overall modified Zagreb index of order 0	Topological indices
89	ON0V	overall modified Zagreb index of order 0 by valence vertex degrees	Topological indices
90	ON1	overall modified Zagreb index of order 1	Topological indices
91	ON1V	overall modified Zagreb index of order 1 by valence vertex degrees	Topological indices
92	Qindex	quadratic index	Topological indices

93	BBI	Bertz branching index	Topological indices
94	DBI	Dragon branching index	Topological indices
95	SNar	Narumi simple topological index (log function)	Topological indices
96	HNar	Narumi harmonic topological index	Topological indices
97	GNar	Narumi geometric topological index	Topological indices
98	Xt	total structure connectivity index	Topological indices
99	Dz	Pogliani index	Topological indices
100	Ram	ramification index	Topological indices
101	BLI	Kier benzene-likeness index	Topological indices
102	Pol	polarity number	Topological indices
103	LPRS	log of product of row sums (PRS)	Topological indices
104	MSD	mean square distance index (Balaban)	Topological indices
105	SPI	superpendent index	Topological indices
106	PJ12	2D Petitjean shape index	Topological indices
107	ECC	eccentricity	Topological indices
108	AECC	average eccentricity	Topological indices
109	DECC	eccentric	Topological indices
110	MDDD	mean distance degree deviation	Topological indices
111	UNIP	unipolarity	Topological indices
112	CENT	centralization	Topological indices
113	VAR	variation	Topological indices
114	ICR	radial centric information index	Topological indices
115	SMTI	Schultz Molecular Topological Index (MTI)	Topological indices
116	SMTIV	Schultz Molecular Topological Index by valence vertex degrees	Topological indices
117	GMTI	Gutman Molecular Topological Index	Topological indices
118	GMTIV	Gutman Molecular Topological Index by valence vertex degrees	Topological indices
119	Xu	Xu index	Topological indices
120	CSI	eccentric connectivity index	Topological indices
121	Wap	all-path Wiener index	Topological indices
122	S1K	1-path Kier alpha-modified shape index	Topological indices
123	S2K	2-path Kier alpha-modified shape index	Topological indices
124	S3K	3-path Kier alpha-modified shape index	Topological indices
125	PHI	Kier flexibility index	Topological indices
126	PW2	path/walk 2 - Randic shape index	Topological indices
127	PW3	path/walk 3 - Randic shape index	Topological indices
128	PW4	path/walk 4 - Randic shape index	Topological indices
129	PW5	path/walk 5 - Randic shape index	Topological indices
130	MAXDN	maximal electrotopological negative variation	Topological indices
131	MAXDP	maximal electrotopological positive variation	Topological indices
132	DELS	molecular electrotopological variation	Topological indices
133	TIE	E-state topological parameter	Topological indices
134	Psi_i_s	intrinsic state pseudoconnectivity index - type S	Topological indices
135	Psi_i_A	intrinsic state pseudoconnectivity index - type S average	Topological indices
136	Psi_i_0	intrinsic state pseudoconnectivity index - type 0	Topological indices
137	Psi_i_1	intrinsic state pseudoconnectivity index - type 1	Topological indices
138	Psi_i_t	intrinsic state pseudoconnectivity index - type T	Topological indices
139	Psi_i_0d	intrinsic state pseudoconnectivity index - type 0d	Topological indices
140	Psi_i_1d	intrinsic state pseudoconnectivity index - type 1d	Topological indices
141	Psi_i_1s	intrinsic state pseudoconnectivity index - type 1s	Topological indices
142	Psi_e_A	electrotopological state pseudoconnectivity index - type S average	Topological indices
143	Psi_e_0	electrotopological state pseudoconnectivity index - type 0	Topological indices
144	Psi_e_1	electrotopological state pseudoconnectivity index - type 1	Topological indices
145	Psi_e_t	electrotopological state pseudoconnectivity index - type T	Topological indices
146	Psi_e_0d	electrotopological state pseudoconnectivity index - type 0d	Topological indices
147	Psi_e_1d	electrotopological state pseudoconnectivity index - type 1d	Topological indices
148	Psi_e_1s	electrotopological state pseudoconnectivity index - type 1s	Topological indices
149	BAC	Balaban centric index	Topological indices
150	LOC	lopping centric index	Topological indices
151	MWC01	molecular walk count of order 1	Walk and path counts
152	MWC02	molecular walk count of order 2	Walk and path counts
153	MWC03	molecular walk count of order 3	Walk and path counts
154	MWC04	molecular walk count of order 4	Walk and path counts
155	MWC05	molecular walk count of order 5	Walk and path counts
156	MWC06	molecular walk count of order 6	Walk and path counts
157	MWC07	molecular walk count of order 7	Walk and path counts
158	MWC08	molecular walk count of order 8	Walk and path counts
159	MWC09	molecular walk count of order 9	Walk and path counts
160	MWC10	molecular walk count of order 10	Walk and path counts
161	SRW02	self-returning walk count of order 2	Walk and path counts
162	SRW03	self-returning walk count of order 3	Walk and path counts
163	SRW04	self-returning walk count of order 4	Walk and path counts
164	SRW05	self-returning walk count of order 5	Walk and path counts
165	SRW06	self-returning walk count of order 6	Walk and path counts
166	SRW07	self-returning walk count of order 7	Walk and path counts
167	SRW08	self-returning walk count of order 8	Walk and path counts
168	SRW09	self-returning walk count of order 9	Walk and path counts
169	SRW10	self-returning walk count of order 10	Walk and path counts
170	MPC01	molecular path count of order 1 (no. of non-H bonds)	Walk and path counts
171	MPC02	molecular path count of order 2 (Gordon-Scantlebury index)	Walk and path counts
172	MPC03	molecular path count of order 3	Walk and path counts
173	MPC04	molecular path count of order 4	Walk and path counts
174	MPC05	molecular path count of order 5	Walk and path counts
175	MPC06	molecular path count of order 6	Walk and path counts
176	MPC07	molecular path count of order 7	Walk and path counts
177	MPC08	molecular path count of order 8	Walk and path counts
178	MPC09	molecular path count of order 9	Walk and path counts
179	MPC10	molecular path count of order 10	Walk and path counts
180	piPC01	molecular multiple path count of order 1	Walk and path counts
181	piPC02	molecular multiple path count of order 2	Walk and path counts
182	piPC03	molecular multiple path count of order 3	Walk and path counts
183	piPC04	molecular multiple path count of order 4	Walk and path counts
184	piPC05	molecular multiple path count of order 5	Walk and path counts
185	piPC06	molecular multiple path count of order 6	Walk and path counts
186	piPC07	molecular multiple path count of order 7	Walk and path counts
187	piPC08	molecular multiple path count of order 8	Walk and path counts
188	piPC09	molecular multiple path count of order 9	Walk and path counts

189	pIPC10	molecular multiple path count of order 10	Walk and path counts
190	TWC	total walk count	Walk and path counts
191	TPC	total path count	Walk and path counts
192	piID	conventional bond order ID number	Walk and path counts
193	PCR	ratio of multiple path count over path count	Walk and path counts
194	PCD	difference between multiple path count and path count	Walk and path counts
195	CID	Randic ID number	Walk and path counts
196	BID	Balaban ID number	Walk and path counts
197	X0	connectivity index of order 0	Connectivity indices
198	X1	connectivity index of order 1 (Randic connectivity index)	Connectivity indices
199	X2	connectivity index of order 2	Connectivity indices
200	X3	connectivity index of order 3	Connectivity indices
201	X4	connectivity index of order 4	Connectivity indices
202	X5	connectivity index of order 5	Connectivity indices
203	X0A	average connectivity index of order 0	Connectivity indices
204	X1A	average connectivity index of order 1	Connectivity indices
205	X2A	average connectivity index of order 2	Connectivity indices
206	X3A	average connectivity index of order 3	Connectivity indices
207	X4A	average connectivity index of order 4	Connectivity indices
208	X5A	average connectivity index of order 5	Connectivity indices
209	X0v	valence connectivity index of order 0	Connectivity indices
210	X1v	valence connectivity index of order 1	Connectivity indices
211	X2v	valence connectivity index of order 2	Connectivity indices
212	X3v	valence connectivity index of order 3	Connectivity indices
213	X4v	valence connectivity index of order 4	Connectivity indices
214	X5v	valence connectivity index of order 5	Connectivity indices
215	X0Av	average valence connectivity index of order 0	Connectivity indices
216	X1Av	average valence connectivity index of order 1	Connectivity indices
217	X2Av	average valence connectivity index of order 2	Connectivity indices
218	X3Av	average valence connectivity index of order 3	Connectivity indices
219	X4Av	average valence connectivity index of order 4	Connectivity indices
220	X5Av	average valence connectivity index of order 5	Connectivity indices
221	X0sol	solvation connectivity index of order 0	Connectivity indices
222	X1sol	solvation connectivity index of order 1	Connectivity indices
223	X2sol	solvation connectivity index of order 2	Connectivity indices
224	X3sol	solvation connectivity index of order 3	Connectivity indices
225	X4sol	solvation connectivity index of order 4	Connectivity indices
226	X5sol	solvation connectivity index of order 5	Connectivity indices
227	XMOD	modified Randic index	Connectivity indices
228	RDCHI	reciprocal distance sum Randic-like index	Connectivity indices
229	RDSQ	reciprocal distance sum inverse Randic-like index	Connectivity indices
230	X1Kup	Kupchik connectivity index	Connectivity indices
231	X1Mad	connectivity topochemical index	Connectivity indices
232	X1Per	perturbation connectivity index	Connectivity indices
233	X1MulPer	multiplicative perturbation connectivity index	Connectivity indices
234	ISIZ	information index on molecular size	Information indices
235	IAC	total information index on atomic composition	Information indices
236	AAC	mean information index on atomic composition	Information indices
237	IDE	mean information content on the distance equality	Information indices
238	IDM	mean information content on the distance magnitude	Information indices
239	IDDE	mean information content on the distance degree equality	Information indices
240	IDDM	mean information content on the distance degree magnitude	Information indices
241	IDET	total information content on the distance equality	Information indices
242	IDMT	total information content on the distance magnitude	Information indices
243	IVDE	mean information content on the vertex degree equality	Information indices
244	IVDM	mean information content on the vertex degree magnitude	Information indices
245	S0K	Kier symmetry index	Information indices
246	HVcpx	graph vertex complexity index	Information indices
247	HDcpx	graph distance complexity index (log function)	Information indices
248	Uindex	Balaban U index	Information indices
249	Vindex	Balaban V index	Information indices
250	Xindex	Balaban X index	Information indices
251	Yindex	Balaban Y index	Information indices
252	IC0	Information Content index (neighborhood symmetry of 0-order)	Information indices
253	IC1	Information Content index (neighborhood symmetry of 1-order)	Information indices
254	IC2	Information Content index (neighborhood symmetry of 2-order)	Information indices
255	IC3	Information Content index (neighborhood symmetry of 3-order)	Information indices
256	IC4	Information Content index (neighborhood symmetry of 4-order)	Information indices
257	IC5	Information Content index (neighborhood symmetry of 5-order)	Information indices
258	TIC0	Total Information Content index (neighborhood symmetry of 0-order)	Information indices
259	TIC1	Total Information Content index (neighborhood symmetry of 1-order)	Information indices
260	TIC2	Total Information Content index (neighborhood symmetry of 2-order)	Information indices
261	TIC3	Total Information Content index (neighborhood symmetry of 3-order)	Information indices
262	TIC4	Total Information Content index (neighborhood symmetry of 4-order)	Information indices
263	TIC5	Total Information Content index (neighborhood symmetry of 5-order)	Information indices
264	SIC0	Structural Information Content index (neighborhood symmetry of 0-order)	Information indices
265	SIC1	Structural Information Content index (neighborhood symmetry of 1-order)	Information indices
266	SIC2	Structural Information Content index (neighborhood symmetry of 2-order)	Information indices
267	SIC3	Structural Information Content index (neighborhood symmetry of 3-order)	Information indices
268	SIC4	Structural Information Content index (neighborhood symmetry of 4-order)	Information indices
269	SIC5	Structural Information Content index (neighborhood symmetry of 5-order)	Information indices
270	CIC0	Complementary Information Content index (neighborhood symmetry of 0-order)	Information indices
271	CIC1	Complementary Information Content index (neighborhood symmetry of 1-order)	Information indices
272	CIC2	Complementary Information Content index (neighborhood symmetry of 2-order)	Information indices
273	CIC3	Complementary Information Content index (neighborhood symmetry of 3-order)	Information indices
274	CIC4	Complementary Information Content index (neighborhood symmetry of 4-order)	Information indices
275	CIC5	Complementary Information Content index (neighborhood symmetry of 5-order)	Information indices
276	BIC0	Bond Information Content index (neighborhood symmetry of 0-order)	Information indices
277	BIC1	Bond Information Content index (neighborhood symmetry of 1-order)	Information indices
278	BIC2	Bond Information Content index (neighborhood symmetry of 2-order)	Information indices
279	BIC3	Bond Information Content index (neighborhood symmetry of 3-order)	Information indices
280	BIC4	Bond Information Content index (neighborhood symmetry of 4-order)	Information indices
281	BIC5	Bond Information Content index (neighborhood symmetry of 5-order)	Information indices
282	J_A	Balaban-like index from adjacency matrix	2D matrix-based descriptors
283	SpPos_A	spectral positive sum from adjacency matrix	2D matrix-based descriptors
284	SpPosA_A	normalized spectral positive sum from adjacency matrix	2D matrix-based descriptors

285	SpPosLog_A	logarithmic spectral positive sum from adjacency matrix	2D matrix-based descriptors
286	SpMax_A	leading eigenvalue from adjacency matrix (Lovasz-Pelikan index)	2D matrix-based descriptors
287	SpMaxA_A	normalized leading eigenvalue from adjacency matrix	2D matrix-based descriptors
288	SpDiam_A	spectral diameter from adjacency matrix	2D matrix-based descriptors
289	SpAD_A	spectral absolute deviation from adjacency matrix	2D matrix-based descriptors
290	SpMAD_A	spectral mean absolute deviation from adjacency matrix	2D matrix-based descriptors
291	Ho_A	Hosoya-like index (log function) from adjacency matrix	2D matrix-based descriptors
292	EE_A	Estrada-like index (log function) from adjacency matrix	2D matrix-based descriptors
293	VE1_A	coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
294	VE2_A	average coefficient of the last eigenvector from adjacency matrix	2D matrix-based descriptors
295	VE3_A	logarithmic coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
296	VR1_A	Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
297	VR2_A	normalized Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
298	VR3_A	logarithmic Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
299	Wi_D	Wiener-like index from topological distance matrix (Wiener index)	2D matrix-based descriptors
300	WiA_D	average Wiener-like index from topological distance matrix	2D matrix-based descriptors
301	AVS_D	average vertex sum from topological distance matrix	2D matrix-based descriptors
302	H_D	Harary-like index from topological distance matrix (Harary index)	2D matrix-based descriptors
303	Chi_D	Randic-like index from topological distance matrix	2D matrix-based descriptors
304	ChiA_D	average Randic-like index from topological distance matrix	2D matrix-based descriptors
305	J_D	Balaban-like index from topological distance matrix (Balaban distance connectivity index)	2D matrix-based descriptors
306	HyWi_D	hyper-Wiener-like index (log function) from topological distance matrix	2D matrix-based descriptors
307	SpPos_D	spectral positive sum from topological distance matrix	2D matrix-based descriptors
308	SpPosA_D	normalized spectral positive sum from topological distance matrix	2D matrix-based descriptors
309	SpPosLog_D	logarithmic spectral positive sum from topological distance matrix	2D matrix-based descriptors
310	SpMax_D	leading eigenvalue from topological distance matrix	2D matrix-based descriptors
311	SpMaxA_D	normalized leading eigenvalue from topological distance matrix	2D matrix-based descriptors
312	SpDiam_D	spectral diameter from topological distance matrix	2D matrix-based descriptors
313	SpAD_D	spectral absolute deviation from topological distance matrix	2D matrix-based descriptors
314	SpMAD_D	spectral mean absolute deviation from topological distance matrix	2D matrix-based descriptors
315	Ho_D	Hosoya-like index (log function) from topological distance matrix	2D matrix-based descriptors
316	EE_D	Estrada-like index (log function) from topological distance matrix	2D matrix-based descriptors
317	SM2_D	spectral moment of order 2 from topological distance matrix	2D matrix-based descriptors
318	SM3_D	spectral moment of order 3 from topological distance matrix	2D matrix-based descriptors
319	SM4_D	spectral moment of order 4 from topological distance matrix	2D matrix-based descriptors
320	SM5_D	spectral moment of order 5 from topological distance matrix	2D matrix-based descriptors
321	SM6_D	spectral moment of order 6 from topological distance matrix	2D matrix-based descriptors
322	VE1_D	coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
323	VE2_D	average coefficient of the last eigenvector from topological distance matrix	2D matrix-based descriptors
324	VE3_D	logarithmic coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
325	VR1_D	Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
326	VR2_D	normalized Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
327	VR3_D	logarithmic Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
328	QW_L	quasi-Wiener index (Kirchhoff number) from Laplace matrix	2D matrix-based descriptors
329	T1_L	first Mohar index from Laplace matrix	2D matrix-based descriptors
330	T2_L	second Mohar index from Laplace matrix	2D matrix-based descriptors
331	STN_L	spanning tree number (log function) from Laplace matrix	2D matrix-based descriptors
332	SpPos_L	spectral positive sum from Laplace matrix	2D matrix-based descriptors
333	SpPosA_L	normalized spectral positive sum from Laplace matrix	2D matrix-based descriptors
334	SpPosLog_L	logarithmic spectral positive sum from Laplace matrix	2D matrix-based descriptors
335	SpMax_L	leading eigenvalue from Laplace matrix	2D matrix-based descriptors
336	SpMaxA_L	normalized leading eigenvalue from Laplace matrix	2D matrix-based descriptors
337	SpDiam_L	spectral diameter from Laplace matrix	2D matrix-based descriptors
338	SpAD_L	spectral absolute deviation from Laplace matrix	2D matrix-based descriptors
339	SpMAD_L	spectral mean absolute deviation from Laplace matrix	2D matrix-based descriptors
340	Ho_L	Hosoya-like index (log function) from Laplace matrix	2D matrix-based descriptors
341	EE_L	Estrada-like index (log function) from Laplace matrix	2D matrix-based descriptors
342	SM2_L	spectral moment of order 2 from Laplace matrix	2D matrix-based descriptors
343	SM3_L	spectral moment of order 3 from Laplace matrix	2D matrix-based descriptors
344	SM4_L	spectral moment of order 4 from Laplace matrix	2D matrix-based descriptors
345	SM5_L	spectral moment of order 5 from Laplace matrix	2D matrix-based descriptors
346	SM6_L	spectral moment of order 6 from Laplace matrix	2D matrix-based descriptors
347	VE1_L	coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
348	VE2_L	average coefficient of the last eigenvector from Laplace matrix	2D matrix-based descriptors
349	VE3_L	logarithmic coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
350	VR1_L	Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
351	VR2_L	normalized Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
352	VR3_L	logarithmic Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
353	AVS_X	average vertex sum from chi matrix	2D matrix-based descriptors
354	H_X	Harary-like index from chi matrix	2D matrix-based descriptors
355	Chi_X	Randic-like index from chi matrix	2D matrix-based descriptors
356	ChiA_X	average Randic-like index from chi matrix	2D matrix-based descriptors
357	J_X	Balaban-like index from chi matrix	2D matrix-based descriptors
358	HyWi_X	hyper-Wiener-like index (log function) from chi matrix	2D matrix-based descriptors
359	SpPos_X	spectral positive sum from chi matrix	2D matrix-based descriptors
360	SpPosA_X	normalized spectral positive sum from chi matrix	2D matrix-based descriptors
361	SpPosLog_X	logarithmic spectral positive sum from chi matrix	2D matrix-based descriptors
362	SpMax_X	leading eigenvalue from chi matrix	2D matrix-based descriptors
363	SpMaxA_X	normalized leading eigenvalue from chi matrix	2D matrix-based descriptors
364	SpDiam_X	spectral diameter from chi matrix	2D matrix-based descriptors
365	SpAD_X	spectral absolute deviation from chi matrix	2D matrix-based descriptors
366	SpMAD_X	spectral mean absolute deviation from chi matrix	2D matrix-based descriptors
367	Ho_X	Hosoya-like index (log function) from chi matrix	2D matrix-based descriptors
368	EE_X	Estrada-like index (log function) from chi matrix	2D matrix-based descriptors
369	SM2_X	spectral moment of order 2 from chi matrix	2D matrix-based descriptors
370	SM3_X	spectral moment of order 3 from chi matrix	2D matrix-based descriptors
371	SM4_X	spectral moment of order 4 from chi matrix	2D matrix-based descriptors
372	SM5_X	spectral moment of order 5 from chi matrix	2D matrix-based descriptors
373	SM6_X	spectral moment of order 6 from chi matrix	2D matrix-based descriptors
374	VE1_X	coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
375	VE2_X	average coefficient of the last eigenvector from chi matrix	2D matrix-based descriptors
376	VE3_X	logarithmic coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
377	VR1_X	Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
378	VR2_X	normalized Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
379	VR3_X	logarithmic Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
380	Wi_H2	Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors



381	WiA_H2	average Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors
382	AVS_H2	average vertex sum from reciprocal squared distance matrix	2D matrix-based descriptors
383	Chi_H2	Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
384	ChiA_H2	average Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
385	J_H2	Balaban-like index from reciprocal squared distance matrix	2D matrix-based descriptors
386	HyWi_H2	hyper-Wiener-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
387	SpPos_H2	spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
388	SpPosA_H2	normalized spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
389	SpPosLog_H2	logarithmic spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
390	SpMax_H2	leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
391	SpMaxA_H2	normalized leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
392	SpDiam_H2	spectral diameter from reciprocal squared distance matrix	2D matrix-based descriptors
393	SpAD_H2	spectral absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors
394	SpMAD_H2	spectral mean absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors
395	Ho_H2	Hosoya-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
396	EE_H2	Estrada-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
397	SM2_H2	spectral moment of order 2 from reciprocal squared distance matrix	2D matrix-based descriptors
398	SM3_H2	spectral moment of order 3 from reciprocal squared distance matrix	2D matrix-based descriptors
399	SM4_H2	spectral moment of order 4 from reciprocal squared distance matrix	2D matrix-based descriptors
400	SM5_H2	spectral moment of order 5 from reciprocal squared distance matrix	2D matrix-based descriptors
401	SM6_H2	spectral moment of order 6 from reciprocal squared distance matrix	2D matrix-based descriptors
402	VE1_H2	coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
403	VE2_H2	average coefficient of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
404	VE3_H2	logarithmic coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
405	VR1_H2	Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
406	VR2_H2	normalized Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
407	VR3_H2	logarithmic Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
408	Wi_Dt	Wiener-like index from detour matrix (detour index)	2D matrix-based descriptors
409	WiA_Dt	average Wiener-like index from detour matrix	2D matrix-based descriptors
410	AVS_Dt	average vertex sum from detour matrix	2D matrix-based descriptors
411	H_Dt	Harary-like index from detour matrix	2D matrix-based descriptors
412	Chi_Dt	Randic-like index from detour matrix	2D matrix-based descriptors
413	ChiA_Dt	average Randic-like index from detour matrix	2D matrix-based descriptors
414	J_Dt	Balaban-like index from detour matrix	2D matrix-based descriptors
415	HyWi_Dt	hyper-Wiener-like index (log function) from detour matrix	2D matrix-based descriptors
416	SpPos_Dt	spectral positive sum from detour matrix	2D matrix-based descriptors
417	SpPosA_Dt	normalized spectral positive sum from detour matrix	2D matrix-based descriptors
418	SpPosLog_Dt	logarithmic spectral positive sum from detour matrix	2D matrix-based descriptors
419	SpMax_Dt	leading eigenvalue from detour matrix	2D matrix-based descriptors
420	SpMaxA_Dt	normalized leading eigenvalue from detour matrix	2D matrix-based descriptors
421	SpDiam_Dt	spectral diameter from detour matrix	2D matrix-based descriptors
422	SpAD_Dt	spectral absolute deviation from detour matrix	2D matrix-based descriptors
423	SpMAD_Dt	spectral mean absolute deviation from detour matrix	2D matrix-based descriptors
424	Ho_Dt	Hosoya-like index (log function) from detour matrix	2D matrix-based descriptors
425	EE_Dt	Estrada-like index (log function) from detour matrix	2D matrix-based descriptors
426	SM2_Dt	spectral moment of order 2 from detour matrix	2D matrix-based descriptors
427	SM3_Dt	spectral moment of order 3 from detour matrix	2D matrix-based descriptors
428	SM4_Dt	spectral moment of order 4 from detour matrix	2D matrix-based descriptors
429	SM5_Dt	spectral moment of order 5 from detour matrix	2D matrix-based descriptors
430	SM6_Dt	spectral moment of order 6 from detour matrix	2D matrix-based descriptors
431	VE1_Dt	coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
432	VE2_Dt	average coefficient of the last eigenvector from detour matrix	2D matrix-based descriptors
433	VE3_Dt	logarithmic coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
434	VR1_Dt	Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
435	VR2_Dt	normalized Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
436	VR3_Dt	logarithmic Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
437	Wi_D/Dt	Wiener-like index from distance/detour matrix	2D matrix-based descriptors
438	WiA_D/Dt	average Wiener-like index from distance/detour matrix	2D matrix-based descriptors
439	AVS_D/Dt	average vertex sum from distance/detour matrix	2D matrix-based descriptors
440	H_D/Dt	Harary-like index from distance/detour matrix	2D matrix-based descriptors
441	Chi_D/Dt	Randic-like index from distance/detour matrix	2D matrix-based descriptors
442	ChiA_D/Dt	average Randic-like index from distance/detour matrix	2D matrix-based descriptors
443	J_D/Dt	Balaban-like index from distance/detour matrix	2D matrix-based descriptors
444	HyWi_D/Dt	hyper-Wiener-like index (log function) from distance/detour matrix	2D matrix-based descriptors
445	SpPos_D/Dt	spectral positive sum from distance/detour matrix	2D matrix-based descriptors
446	SpPosA_D/Dt	normalized spectral positive sum from distance/detour matrix	2D matrix-based descriptors
447	SpPosLog_D/Dt	logarithmic spectral positive sum from distance/detour matrix	2D matrix-based descriptors
448	SpMax_D/Dt	leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
449	SpMaxA_D/Dt	normalized leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
450	SpDiam_D/Dt	spectral diameter from distance/detour matrix	2D matrix-based descriptors
451	SpAD_D/Dt	spectral absolute deviation from distance/detour matrix	2D matrix-based descriptors
452	SpMAD_D/Dt	spectral mean absolute deviation from distance/detour matrix	2D matrix-based descriptors
453	Ho_D/Dt	Hosoya-like index (log function) from distance/detour matrix	2D matrix-based descriptors
454	EE_D/Dt	Estrada-like index (log function) from distance/detour matrix	2D matrix-based descriptors
455	SM2_D/Dt	spectral moment of order 2 from distance/detour matrix	2D matrix-based descriptors
456	SM3_D/Dt	spectral moment of order 3 from distance/detour matrix	2D matrix-based descriptors
457	SM4_D/Dt	spectral moment of order 4 from distance/detour matrix	2D matrix-based descriptors
458	SM5_D/Dt	spectral moment of order 5 from distance/detour matrix	2D matrix-based descriptors
459	SM6_D/Dt	spectral moment of order 6 from distance/detour matrix	2D matrix-based descriptors
460	VE1_D/Dt	coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
461	VE2_D/Dt	average coefficient of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
462	VE3_D/Dt	logarithmic coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
463	VR1_D/Dt	Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
464	VR2_D/Dt	normalized Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
465	VR3_D/Dt	logarithmic Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
466	Wi_Dz(Z)	Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
467	WiA_Dz(Z)	average Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
468	AVS_Dz(Z)	average vertex sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
469	H_Dz(Z)	Harary-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
470	Chi_Dz(Z)	Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
471	ChiA_Dz(Z)	average Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
472	J_Dz(Z)	Balaban-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
473	HyWi_Dz(Z)	hyper-Wiener-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
474	SpAbs_Dz(Z)	graph energy from Barysz matrix weighted by atomic number	2D matrix-based descriptors
475	SpPos_Dz(Z)	spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
476	SpPosA_Dz(Z)	normalized spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors























1149	P_VSA_MR_1	P_VSA-like on Molar Refractivity, bin 1	P_VSA-like descriptors
1150	P_VSA_MR_2	P_VSA-like on Molar Refractivity, bin 2	P_VSA-like descriptors
1151	P_VSA_MR_3	P_VSA-like on Molar Refractivity, bin 3	P_VSA-like descriptors
1152	P_VSA_MR_4	P_VSA-like on Molar Refractivity, bin 4	P_VSA-like descriptors
1153	P_VSA_MR_5	P_VSA-like on Molar Refractivity, bin 5	P_VSA-like descriptors
1154	P_VSA_MR_6	P_VSA-like on Molar Refractivity, bin 6	P_VSA-like descriptors
1155	P_VSA_MR_7	P_VSA-like on Molar Refractivity, bin 7	P_VSA-like descriptors
1156	P_VSA_MR_8	P_VSA-like on Molar Refractivity, bin 8	P_VSA-like descriptors
1157	P_VSA_m_1	P_VSA-like on mass, bin 1	P_VSA-like descriptors
1158	P_VSA_m_2	P_VSA-like on mass, bin 2	P_VSA-like descriptors
1159	P_VSA_m_3	P_VSA-like on mass, bin 3	P_VSA-like descriptors
1160	P_VSA_m_4	P_VSA-like on mass, bin 4	P_VSA-like descriptors
1161	P_VSA_m_5	P_VSA-like on mass, bin 5	P_VSA-like descriptors
1162	P_VSA_v_1	P_VSA-like on van der Waals volume, bin 1	P_VSA-like descriptors
1163	P_VSA_v_2	P_VSA-like on van der Waals volume, bin 2	P_VSA-like descriptors
1164	P_VSA_v_3	P_VSA-like on van der Waals volume, bin 3	P_VSA-like descriptors
1165	P_VSA_v_4	P_VSA-like on van der Waals volume, bin 4	P_VSA-like descriptors
1166	P_VSA_e_1	P_VSA-like on Sanderson electronegativity, bin 1	P_VSA-like descriptors
1167	P_VSA_e_2	P_VSA-like on Sanderson electronegativity, bin 2	P_VSA-like descriptors
1168	P_VSA_e_3	P_VSA-like on Sanderson electronegativity, bin 3	P_VSA-like descriptors
1169	P_VSA_e_4	P_VSA-like on Sanderson electronegativity, bin 4	P_VSA-like descriptors
1170	P_VSA_e_5	P_VSA-like on Sanderson electronegativity, bin 5	P_VSA-like descriptors
1171	P_VSA_e_6	P_VSA-like on Sanderson electronegativity, bin 6	P_VSA-like descriptors
1172	P_VSA_p_1	P_VSA-like on polarizability, bin 1	P_VSA-like descriptors
1173	P_VSA_p_2	P_VSA-like on polarizability, bin 2	P_VSA-like descriptors
1174	P_VSA_p_3	P_VSA-like on polarizability, bin 3	P_VSA-like descriptors
1175	P_VSA_p_4	P_VSA-like on polarizability, bin 4	P_VSA-like descriptors
1176	P_VSA_i_1	P_VSA-like on ionization potential, bin 1	P_VSA-like descriptors
1177	P_VSA_i_2	P_VSA-like on ionization potential, bin 2	P_VSA-like descriptors
1178	P_VSA_i_3	P_VSA-like on ionization potential, bin 3	P_VSA-like descriptors
1179	P_VSA_i_4	P_VSA-like on ionization potential, bin 4	P_VSA-like descriptors
1180	P_VSA_s_1	P_VSA-like on l-state, bin 1	P_VSA-like descriptors
1181	P_VSA_s_2	P_VSA-like on l-state, bin 2	P_VSA-like descriptors
1182	P_VSA_s_3	P_VSA-like on l-state, bin 3	P_VSA-like descriptors
1183	P_VSA_s_4	P_VSA-like on l-state, bin 4	P_VSA-like descriptors
1184	P_VSA_s_5	P_VSA-like on l-state, bin 5	P_VSA-like descriptors
1185	P_VSA_s_6	P_VSA-like on l-state, bin 6	P_VSA-like descriptors
1186	Eta_alpha	eta core count	ETA indices
1187	Eta_alpha_A	eta average core count	ETA indices
1188	Eta_epsi	eta electronegativity measure	ETA indices
1189	Eta_epsi_A	eta average electronegativity measure	ETA indices
1190	Eta_betaS	eta sigma VEM count	ETA indices
1191	Eta_betaS_A	eta sigma average VEM coun	ETA indices
1192	Eta_betaP	eta pi and lone pair VEM count	ETA indices
1193	Eta_betaP_A	eta pi and lone pair average VEM count	ETA indices
1194	Eta_beta	eta VEM count	ETA indices
1195	Eta_beta_A	eta average VEM count	ETA indices
1196	Eta_C	eta composite index	ETA indices
1197	Eta_C_A	eta average composite index	ETA indices
1198	Eta_L	eta local composite index	ETA indices
1199	Eta_L_A	eta average local composite index	ETA indices
1200	Eta_F	eta functionality index	ETA indices
1201	Eta_F_A	eta average functionality index	ETA indices
1202	Eta_FL	eta local functionality index	ETA indices
1203	Eta_FL_A	eta average local functionality index	ETA indices
1204	Eta_B	eta branching index	ETA indices
1205	Eta_B_A	eta average branching index	ETA indices
1206	Eta_sh_p	eta p shape index	ETA indices
1207	Eta_sh_y	eta y shape index	ETA indices
1208	Eta_sh_x	eta x shape index	ETA indices
1209	SpMax_EA	leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1210	SpMaxA_EA	normalized leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1211	SpDiam_EA	spectral diameter from edge adjacency mat.	Edge adjacency indices
1212	SpAD_EA	spectral absolute deviation from edge adjacency mat.	Edge adjacency indices
1213	SpMAD_EA	spectral mean absolute deviation from edge adjacency mat.	Edge adjacency indices
1214	SpMax_EA(ed)	leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1215	SpMaxA_EA(ed)	normalized leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1216	SpDiam_EA(ed)	spectral diameter from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1217	SpAD_EA(ed)	spectral absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1218	SpMAD_EA(ed)	spectral mean absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1219	SpMax_EA(bo)	leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices
1220	SpMaxA_EA(bo)	normalized leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices
1221	SpDiam_EA(bo)	spectral diameter from edge adjacency mat. weighted by bond order	Edge adjacency indices
1222	SpAD_EA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices
1223	SpMAD_EA(bo)	spectral mean absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices
1224	SpMax_EA(dm)	leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1225	SpMaxA_EA(dm)	normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1226	SpDiam_EA(dm)	spectral diameter from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1227	SpAD_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1228	SpMAD_EA(dm)	spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1229	SpMax_EA(ri)	leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1230	SpMaxA_EA(ri)	normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1231	SpDiam_EA(ri)	spectral diameter from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1232	SpAD_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1233	SpMAD_EA(ri)	spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1234	SpMax_AEA(ed)	leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1235	SpMaxA_AEA(ed)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1236	SpDiam_AEA(ed)	spectral diameter from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1237	SpAD_AEA(ed)	spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1238	SpMAD_AEA(ed)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1239	SpMax_AEA(bo)	leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1240	SpMaxA_AEA(bo)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1241	SpDiam_AEA(bo)	spectral diameter from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1242	SpAD_AEA(bo)	spectral absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1243	SpMAD_AEA(bo)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1244	SpMax_AEA(dm)	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices











1533	G1	gravitational index G1	Geometrical descriptors
1534	G2	gravitational index G2 (bond-restricted)	Geometrical descriptors
1535	RGyr	radius of gyration (mass weighted)	Geometrical descriptors
1536	SPAN	span R	Geometrical descriptors
1537	SPAM	average span R	Geometrical descriptors
1538	MEcc	molecular eccentricity	Geometrical descriptors
1539	SPH	sphericity	Geometrical descriptors
1540	ASP	asphericity	Geometrical descriptors
1541	PJl3	3D Petitjean shape index	Geometrical descriptors
1542	L/Bw	length-to-breadth ratio by WHIM	Geometrical descriptors
1543	HOMA	Harmonic Oscillator Model of Aromaticity index	Geometrical descriptors
1544	CMBL	conjugated maximum bond length	Geometrical descriptors
1545	AROM	aromaticity index	Geometrical descriptors
1546	HOMT	HOMA total	Geometrical descriptors
1547	DISPm	displacement value / weighted by mass	Geometrical descriptors
1548	QXXm	quadrupole x-component value / weighted by mass	Geometrical descriptors
1549	QYYm	quadrupole y-component value / weighted by mass	Geometrical descriptors
1550	QZZm	quadrupole z-component value / weighted by mass	Geometrical descriptors
1551	DISPv	displacement value / weighted by van der Waals volume	Geometrical descriptors
1552	QXXv	quadrupole x-component value / weighted by van der Waals volume	Geometrical descriptors
1553	QYYv	quadrupole y-component value / weighted by van der Waals volume	Geometrical descriptors
1554	QZZv	quadrupole z-component value / weighted by van der Waals volume	Geometrical descriptors
1555	DISPe	displacement value / weighted by Sanderson electronegativity	Geometrical descriptors
1556	QXXe	quadrupole x-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1557	QYYe	quadrupole y-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1558	QZZe	quadrupole z-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1559	DISPp	displacement value / weighted by polarizability	Geometrical descriptors
1560	QXXp	quadrupole x-component value / weighted by polarizability	Geometrical descriptors
1561	QYYp	quadrupole y-component value / weighted by polarizability	Geometrical descriptors
1562	QZZp	quadrupole z-component value / weighted by polarizability	Geometrical descriptors
1563	DISPi	displacement value / weighted by ionization potential	Geometrical descriptors
1564	QXXi	quadrupole x-component value / weighted by ionization potential	Geometrical descriptors
1565	QYYi	quadrupole y-component value / weighted by ionization potential	Geometrical descriptors
1566	QZZi	quadrupole z-component value / weighted by ionization potential	Geometrical descriptors
1567	DISPs	displacement value / weighted by I-state	Geometrical descriptors
1568	QXXs	quadrupole x-component value / weighted by I-state	Geometrical descriptors
1569	QYYs	quadrupole y-component value / weighted by I-state	Geometrical descriptors
1570	QZZs	quadrupole z-component value / weighted by I-state	Geometrical descriptors
1571	Wi_G	Wiener-like index from geometrical matrix	3D matrix-based descriptors
1572	WiA_G	average Wiener-like index from geometrical matrix	3D matrix-based descriptors
1573	AVS_G	average vertex sum from geometrical matrix	3D matrix-based descriptors
1574	H_G	Harary-like index from geometrical matrix	3D matrix-based descriptors
1575	Chi_G	Randic-like index from geometrical matrix	3D matrix-based descriptors
1576	ChiA_G	average Randic-like index from geometrical matrix	3D matrix-based descriptors
1577	J_G	Balaban-like index from geometrical matrix	3D matrix-based descriptors
1578	HyWi_G	hyper-Wiener-like index from geometrical matrix	3D matrix-based descriptors
1579	SpAbs_G	graph energy from geometrical matrix	3D matrix-based descriptors
1580	SpPos_G	spectral positive sum from geometrical matrix	3D matrix-based descriptors
1581	SpPosA_G	normalized spectral positive sum from geometrical matrix	3D matrix-based descriptors
1582	SpPosLog_G	logarithmic spectral positive sum from geometrical matrix	3D matrix-based descriptors
1583	SpMax_G	leading eigenvalue from geometrical matrix	3D matrix-based descriptors
1584	SpMaxA_G	normalized leading eigenvalue from geometrical matrix	3D matrix-based descriptors
1585	SpDiam_G	spectral diameter from geometrical matrix	3D matrix-based descriptors
1586	SpAD_G	spectral absolute deviation from geometrical matrix	3D matrix-based descriptors
1587	SpMAD_G	spectral mean absolute deviation from geometrical matrix	3D matrix-based descriptors
1588	Ho_G	Hosoya-like index (log function) from geometrical matrix	3D matrix-based descriptors
1589	EE_G	Estrada-like index (log function) from geometrical matrix	3D matrix-based descriptors
1590	SM2_G	spectral moment of order 2 from geometrical matrix	3D matrix-based descriptors
1591	SM3_G	spectral moment of order 3 from geometrical matrix	3D matrix-based descriptors
1592	SM4_G	spectral moment of order 4 from geometrical matrix	3D matrix-based descriptors
1593	SM5_G	spectral moment of order 5 from geometrical matrix	3D matrix-based descriptors
1594	SM6_G	spectral moment of order 6 from geometrical matrix	3D matrix-based descriptors
1595	VE1_G	coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1596	VE2_G	average coefficient of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1597	VE3_G	logarithmic coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1598	VR1_G	Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1599	VR2_G	normalized Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1600	VR3_G	logarithmic Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1601	Wi_RG	Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1602	WiA_RG	average Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1603	AVS_RG	average vertex sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1604	H_RG	Harary-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1605	Chi_RG	Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1606	ChiA_RG	average Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1607	J_RG	Balaban-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1608	HyWi_RG	hyper-Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1609	SpAbs_RG	graph energy from reciprocal squared geometrical matrix	3D matrix-based descriptors
1610	SpPos_RG	spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1611	SpPosA_RG	normalized spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1612	SpPosLog_RG	logarithmic spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1613	SpMax_RG	leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors
1614	SpMaxA_RG	normalized leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors
1615	SpDiam_RG	spectral diameter from reciprocal squared geometrical matrix	3D matrix-based descriptors
1616	SpAD_RG	spectral absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors
1617	SpMAD_RG	spectral mean absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors
1618	Ho_RG	Hosoya-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1619	EE_RG	Estrada-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1620	SM2_RG	spectral moment of order 2 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1621	SM3_RG	spectral moment of order 3 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1622	SM4_RG	spectral moment of order 4 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1623	SM5_RG	spectral moment of order 5 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1624	SM6_RG	spectral moment of order 6 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1625	VE1_RG	coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1626	VE2_RG	average coefficient of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1627	VE3_RG	logarithmic coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1628	VR1_RG	Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors















2205 E1v	1st component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2206 E2v	2nd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2207 E3v	3rd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2208 L1e	1st component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2209 L2e	2nd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2210 L3e	3rd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2211 P1e	1st component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2212 P2e	2nd component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2213 G1e	1st component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2214 G2e	2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2215 G3e	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2216 E1e	1st component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2217 E2e	2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2218 E3e	3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2219 L1p	1st component size directional WHIM index / weighted by polarizability	WHIM descriptors
2220 L2p	2nd component size directional WHIM index / weighted by polarizability	WHIM descriptors
2221 L3p	3rd component size directional WHIM index / weighted by polarizability	WHIM descriptors
2222 P1p	1st component shape directional WHIM index / weighted by polarizability	WHIM descriptors
2223 P2p	2nd component shape directional WHIM index / weighted by polarizability	WHIM descriptors
2224 G1p	1st component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2225 G2p	2nd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2226 G3p	3rd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2227 E1p	1st component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2228 E2p	2nd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2229 E3p	3rd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2230 L1i	1st component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2231 L2i	2nd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2232 L3i	3rd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2233 P1i	1st component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
2234 P2i	2nd component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
2235 G1i	1st component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2236 G2i	2nd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2237 G3i	3rd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2238 E1i	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2239 E2i	2nd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2240 E3i	3rd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2241 L1s	1st component size directional WHIM index / weighted by I-state	WHIM descriptors
2242 L2s	2nd component size directional WHIM index / weighted by I-state	WHIM descriptors
2243 L3s	3rd component size directional WHIM index / weighted by I-state	WHIM descriptors
2244 P1s	1st component shape directional WHIM index / weighted by I-state	WHIM descriptors
2245 P2s	2nd component shape directional WHIM index / weighted by I-state	WHIM descriptors
2246 G1s	1st component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2247 G2s	2nd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2248 G3s	3rd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2249 E1s	1st component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2250 E2s	2nd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2251 E3s	3rd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2252 Tu	T total size index / unweighted	WHIM descriptors
2253 Tm	T total size index / weighted by mass	WHIM descriptors
2254 Tv	T total size index / weighted by van der Waals volume	WHIM descriptors
2255 Te	T total size index / weighted by Sanderson electronegativity	WHIM descriptors
2256 Tp	T total size index / weighted by polarizability	WHIM descriptors
2257 Ti	T total size index / weighted by ionization potential	WHIM descriptors
2258 Ts	T total size index / weighted by I-state	WHIM descriptors
2259 Au	A total size index / unweighted	WHIM descriptors
2260 Am	A total size index / weighted by mass	WHIM descriptors
2261 Av	A total size index / weighted by van der Waals volume	WHIM descriptors
2262 Ae	A total size index / weighted by Sanderson electronegativity	WHIM descriptors
2263 Ap	A total size index / weighted by polarizability	WHIM descriptors
2264 Ai	A total size index / weighted by ionization potential	WHIM descriptors
2265 As	A total size index / weighted by I-state	WHIM descriptors
2266 Gu	total symmetry index / unweighted	WHIM descriptors
2267 Gm	total symmetry index / weighted by mass	WHIM descriptors
2268 Ku	K global shape index / unweighted	WHIM descriptors
2269 Km	K global shape index / weighted by mass	WHIM descriptors
2270 Kv	K global shape index / weighted by van der Waals volume	WHIM descriptors
2271 Ke	K global shape index / weighted by Sanderson electronegativity	WHIM descriptors
2272 Kp	K global shape index / weighted by polarizability	WHIM descriptors
2273 Ki	K global shape index / weighted by ionization potential	WHIM descriptors
2274 Ks	K global shape index / weighted by I-state	WHIM descriptors
2275 Du	D total accessibility index / unweighted	WHIM descriptors
2276 Dm	D total accessibility index / weighted by mass	WHIM descriptors
2277 Dv	D total accessibility index / weighted by van der Waals volume	WHIM descriptors
2278 De	D total accessibility index / weighted by Sanderson electronegativity	WHIM descriptors
2279 Dp	D total accessibility index / weighted by polarizability	WHIM descriptors
2280 Di	D total accessibility index / weighted by ionization potential	WHIM descriptors
2281 Ds	D total accessibility index / weighted by I-state	WHIM descriptors
2282 Vu	V total size index / unweighted	WHIM descriptors
2283 Vm	V total size index / weighted by mass	WHIM descriptors
2284 Vv	V total size index / weighted by van der Waals volume	WHIM descriptors
2285 Ve	V total size index / weighted by Sanderson electronegativity	WHIM descriptors
2286 Vp	V total size index / weighted by polarizability	WHIM descriptors
2287 Vi	V total size index / weighted by ionization potential	WHIM descriptors
2288 Vs	V total size index / weighted by I-state	WHIM descriptors
2289 ITH	total information content on the leverage equality	GETAWAY descriptors
2290 ISH	standardized information content on the leverage equality	GETAWAY descriptors
2291 HIC	mean information content on the leverage magnitude	GETAWAY descriptors
2292 HGM	geometric mean on the leverage magnitude	GETAWAY descriptors
2293 H0u	H autocorrelation of lag 0 / unweighted	GETAWAY descriptors
2294 H1u	H autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2295 H2u	H autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2296 H3u	H autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2297 H4u	H autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2298 H5u	H autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2299 H6u	H autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2300 H7u	H autocorrelation of lag 7 / unweighted	GETAWAY descriptors





2397 H4i	H autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2398 H5i	H autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2399 H6i	H autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2400 H7i	H autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2401 H8i	H autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2402 HTi	H total index / weighted by ionization potential	GETAWAY descriptors
2403 HATS0i	leverage-weighted autocorrelation of lag 0 / weighted by ionization potential	GETAWAY descriptors
2404 HATS1i	leverage-weighted autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2405 HATS2i	leverage-weighted autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2406 HATS3i	leverage-weighted autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2407 HATS4i	leverage-weighted autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2408 HATS5i	leverage-weighted autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2409 HATS6i	leverage-weighted autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2410 HATS7i	leverage-weighted autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2411 HATS8i	leverage-weighted autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2412 HATSi	leverage-weighted total index / weighted by ionization potential	GETAWAY descriptors
2413 H0s	H autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors
2414 H1s	H autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2415 H2s	H autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2416 H3s	H autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2417 H4s	H autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2418 H5s	H autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2419 H6s	H autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2420 H7s	H autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2421 H8s	H autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2422 HTs	H total index / weighted by I-state	GETAWAY descriptors
2423 HATS0s	leverage-weighted autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors
2424 HATS1s	leverage-weighted autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2425 HATS2s	leverage-weighted autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2426 HATS3s	leverage-weighted autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2427 HATS4s	leverage-weighted autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2428 HATS5s	leverage-weighted autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2429 HATS6s	leverage-weighted autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2430 HATS7s	leverage-weighted autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2431 HATS8s	leverage-weighted autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2432 HATSs	leverage-weighted total index / weighted by I-state	GETAWAY descriptors
2433 RCON	Randic-type R matrix connectivity	GETAWAY descriptors
2434 RARS	R matrix average row sum	GETAWAY descriptors
2435 REIG	first eigenvalue of the R matrix	GETAWAY descriptors
2436 R1u	R autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2437 R2u	R autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2438 R3u	R autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2439 R4u	R autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2440 R5u	R autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2441 R6u	R autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2442 R7u	R autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2443 R8u	R autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2444 RTu	R total index / unweighted	GETAWAY descriptors
2445 R1u+	R maximal autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2446 R2u+	R maximal autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2447 R3u+	R maximal autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2448 R4u+	R maximal autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2449 R5u+	R maximal autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2450 R6u+	R maximal autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2451 R7u+	R maximal autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2452 R8u+	R maximal autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2453 RTu+	R maximal index / unweighted	GETAWAY descriptors
2454 R1m	R autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2455 R2m	R autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2456 R3m	R autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2457 R4m	R autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors
2458 R5m	R autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2459 R6m	R autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2460 R7m	R autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors
2461 R8m	R autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2462 RTm	R total index / weighted by mass	GETAWAY descriptors
2463 R1m+	R maximal autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2464 R2m+	R maximal autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2465 R3m+	R maximal autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2466 R4m+	R maximal autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors
2467 R5m+	R maximal autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2468 R6m+	R maximal autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2469 R7m+	R maximal autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors
2470 R8m+	R maximal autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2471 RTm+	R maximal index / weighted by mass	GETAWAY descriptors
2472 R1v	R autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2473 R2v	R autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2474 R3v	R autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors
2475 R4v	R autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2476 R5v	R autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2477 R6v	R autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2478 R7v	R autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2479 R8v	R autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors
2480 RTv	R total index / weighted by van der Waals volume	GETAWAY descriptors
2481 R1v+	R maximal autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2482 R2v+	R maximal autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2483 R3v+	R maximal autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors
2484 R4v+	R maximal autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2485 R5v+	R maximal autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2486 R6v+	R maximal autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2487 R7v+	R maximal autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2488 R8v+	R maximal autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors
2489 RTv+	R maximal index / weighted by van der Waals volume	GETAWAY descriptors
2490 R1e	R autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2491 R2e	R autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors
2492 R3e	R autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors



2589	SP08	shape profile no. 8	Randic molecular profiles
2590	SP09	shape profile no. 9	Randic molecular profiles
2591	SP10	shape profile no. 10	Randic molecular profiles
2592	SP11	shape profile no. 11	Randic molecular profiles
2593	SP12	shape profile no. 12	Randic molecular profiles
2594	SP13	shape profile no. 13	Randic molecular profiles
2595	SP14	shape profile no. 14	Randic molecular profiles
2596	SP15	shape profile no. 15	Randic molecular profiles
2597	SP16	shape profile no. 16	Randic molecular profiles
2598	SP17	shape profile no. 17	Randic molecular profiles
2599	SP18	shape profile no. 18	Randic molecular profiles
2600	SP19	shape profile no. 19	Randic molecular profiles
2601	SP20	shape profile no. 20	Randic molecular profiles
2602	SHP2	average shape profile index of order 2	Randic molecular profiles
2603	nCp	number of terminal primary C(sp <sup>3</sup> )	Functional group counts
2604	nCs	number of total secondary C(sp <sup>3</sup> )	Functional group counts
2605	nCt	number of total tertiary C(sp <sup>3</sup> )	Functional group counts
2606	nCq	number of total quaternary C(sp <sup>3</sup> )	Functional group counts
2607	nCr <sub>s</sub>	number of ring secondary C(sp <sup>3</sup> )	Functional group counts
2608	nCr <sub>t</sub>	number of ring tertiary C(sp <sup>3</sup> )	Functional group counts
2609	nCr <sub>q</sub>	number of ring quaternary C(sp <sup>3</sup> )	Functional group counts
2610	nCar	number of aromatic C(sp <sup>2</sup> )	Functional group counts
2611	nCbH	number of unsubstituted benzene C(sp <sup>2</sup> )	Functional group counts
2612	nCb-	number of substituted benzene C(sp <sup>2</sup> )	Functional group counts
2613	nCconj	number of non-aromatic conjugated C(sp <sup>2</sup> )	Functional group counts
2614	nR=Cp	number of terminal primary C(sp <sup>2</sup> )	Functional group counts
2615	nR=C <sub>s</sub>	number of aliphatic secondary C(sp <sup>2</sup> )	Functional group counts
2616	nR=C <sub>t</sub>	number of aliphatic tertiary C(sp <sup>2</sup> )	Functional group counts
2617	n=C=	number of allenes groups	Functional group counts
2618	nR#CH/X	number of terminal C(sp)	Functional group counts
2619	nR#C-	number of non-terminal C(sp)	Functional group counts
2620	nROCN	number of cyanates (aliphatic)	Functional group counts
2621	nArOCN	number of cyanates (aromatic)	Functional group counts
2622	nRNCO	number of isocyanates (aliphatic)	Functional group counts
2623	nArNCO	number of isocyanates (aromatic)	Functional group counts
2624	nRSCN	number of thiocyanates (aliphatic)	Functional group counts
2625	nArSCN	number of thiocyanates (aromatic)	Functional group counts
2626	nRNCS	number of isothiocyanates (aliphatic)	Functional group counts
2627	nArNCS	number of isothiocyanates (aromatic)	Functional group counts
2628	nRCOOH	number of carboxylic acids (aliphatic)	Functional group counts
2629	nArCOOH	number of carboxylic acids (aromatic)	Functional group counts
2630	nRCOOR	number of esters (aliphatic)	Functional group counts
2631	nArCOOR	number of esters (aromatic)	Functional group counts
2632	nRCONH <sub>2</sub>	number of primary amides (aliphatic)	Functional group counts
2633	nArCONH <sub>2</sub>	number of primary amides (aromatic)	Functional group counts
2634	nRCONHR	number of secondary amides (aliphatic)	Functional group counts
2635	nArCONHR	number of secondary amides (aromatic)	Functional group counts
2636	nRCONR <sub>2</sub>	number of tertiary amides (aliphatic)	Functional group counts
2637	nArCONR <sub>2</sub>	number of tertiary amides (aromatic)	Functional group counts
2638	nROCON	number of (thio-) carbamates (aliphatic)	Functional group counts
2639	nArOCON	number of (thio-) carbamates (aromatic)	Functional group counts
2640	nRCOX	number of acyl halogenides (aliphatic)	Functional group counts
2641	nArCOX	number of acyl halogenides (aromatic)	Functional group counts
2642	nRCSOH	number of thioacids (aliphatic)	Functional group counts
2643	nArCSOH	number of thioacids (aromatic)	Functional group counts
2644	nRCSSH	number of dithioacids (aliphatic)	Functional group counts
2645	nArCSSH	number of dithioacids (aromatic)	Functional group counts
2646	nRCOSR	number of thioesters (aliphatic)	Functional group counts
2647	nArCOSR	number of thioesters (aromatic)	Functional group counts
2648	nRCSSR	number of dithioesters (aliphatic)	Functional group counts
2649	nArCSSR	number of dithioesters (aromatic)	Functional group counts
2650	nRCHO	number of aldehydes (aliphatic)	Functional group counts
2651	nArCHO	number of aldehydes (aromatic)	Functional group counts
2652	nRCO	number of ketones (aliphatic)	Functional group counts
2653	nArCO	number of ketones (aromatic)	Functional group counts
2654	nCONN	number of urea (-thio) derivatives	Functional group counts
2655	nC=O(O) <sub>2</sub>	number of carbonate (-thio) derivatives	Functional group counts
2656	nN=C-N<	number of amidine derivatives	Functional group counts
2657	nC(=N) <sub>2</sub>	number of guanidine derivatives	Functional group counts
2658	nRC=N	number of imines (aliphatic)	Functional group counts
2659	nArC=N	number of imines (aromatic)	Functional group counts
2660	nRCNO	number of oximes (aliphatic)	Functional group counts
2661	nArCNO	number of oximes (aromatic)	Functional group counts
2662	nRNH <sub>2</sub>	number of primary amines (aliphatic)	Functional group counts
2663	nArNH <sub>2</sub>	number of primary amines (aromatic)	Functional group counts
2664	nRNHR	number of secondary amines (aliphatic)	Functional group counts
2665	nArNHR	number of secondary amines (aromatic)	Functional group counts
2666	nRNR <sub>2</sub>	number of tertiary amines (aliphatic)	Functional group counts
2667	nArNR <sub>2</sub>	number of tertiary amines (aromatic)	Functional group counts
2668	nN-N	number of N hydrazines	Functional group counts
2669	nN=N	number of N azo-derivatives	Functional group counts
2670	nRCN	number of nitriles (aliphatic)	Functional group counts
2671	nArCN	number of nitriles (aromatic)	Functional group counts
2672	nN+	number of positively charged N	Functional group counts
2673	nNq	number of quaternary N	Functional group counts
2674	nRNHO	number of hydroxylamines (aliphatic)	Functional group counts
2675	nArNHO	number of hydroxylamines (aromatic)	Functional group counts
2676	nRNN <sub>2</sub>	number of N-nitroso groups (aliphatic)	Functional group counts
2677	nArNN <sub>2</sub>	number of N-nitroso groups (aromatic)	Functional group counts
2678	nRNO	number of nitroso groups (aliphatic)	Functional group counts
2679	nArNO	number of nitroso groups (aromatic)	Functional group counts
2680	nRNO <sub>2</sub>	number of nitro groups (aliphatic)	Functional group counts
2681	nArNO <sub>2</sub>	number of nitro groups (aromatic)	Functional group counts
2682	nN(CO) <sub>2</sub>	number of imides (-thio)	Functional group counts
2683	nC=N-N<	number of hydrazones	Functional group counts
2684	nROH	number of hydroxyl groups	Functional group counts



2685 nArOH	number of aromatic hydroxyls	Functional group counts
2686 nOHp	number of primary alcohols	Functional group counts
2687 nOHs	number of secondary alcohols	Functional group counts
2688 nOHt	number of tertiary alcohols	Functional group counts
2689 nROR	number of ethers (aliphatic)	Functional group counts
2690 nArOR	number of ethers (aromatic)	Functional group counts
2691 nROX	number of hypohalogenides (aliphatic)	Functional group counts
2692 nArOX	number of hypohalogenides (aromatic)	Functional group counts
2693 nO(C=O)2	number of anhydrides (-thio)	Functional group counts
2694 nH2O	number of water molecules	Functional group counts
2695 nSH	number of thiols	Functional group counts
2696 nC=S	number of thioketones	Functional group counts
2697 nRSR	number of sulfides	Functional group counts
2698 nRSSR	number of disulfides	Functional group counts
2699 nSO	number of sulfoxides	Functional group counts
2700 nS(=O)2	number of sulfones	Functional group counts
2701 nSOH	number of sulfenic (thio-) acids	Functional group counts
2702 nSOOH	number of sulfinic (thio-/dithio-) acids	Functional group counts
2703 nSO2OH	number of sulfonic (thio-/dithio-) acids	Functional group counts
2704 nSO3OH	number of sulfuric (thio-/dithio-) acids	Functional group counts
2705 nSO2	number of sulfites (thio-/dithio-)	Functional group counts
2706 nSO3	number of sulfonates (thio-/dithio-)	Functional group counts
2707 nSO4	number of sulfates (thio-/dithio-)	Functional group counts
2708 nSO2N	number of sulfonamides (thio-/dithio-)	Functional group counts
2709 nPO3	number of phosphites/thiophosphites	Functional group counts
2710 nPO4	number of phosphates/thiophosphates	Functional group counts
2711 nPR3	number of phosphanes	Functional group counts
2712 nP(=O)O2R	number of phosphonates (thio-)	Functional group counts
2713 nP(=O)R3/nPR5	number of phosphoranes (thio-)	Functional group counts
2714 nCH2RX	number of CHR2X	Functional group counts
2715 nCHR2X	number of CHR2X	Functional group counts
2716 nCR3X	number of CR3X	Functional group counts
2717 nR=CHX	number of R=CHX	Functional group counts
2718 nR=CRX	number of R=CRX	Functional group counts
2719 nR#CX	number of R#CX	Functional group counts
2720 nCHRX2	number of CHRX2	Functional group counts
2721 nCR2X2	number of CR2X2	Functional group counts
2722 nR=CX2	number of R=CX2	Functional group counts
2723 nCRX3	number of CRX3	Functional group counts
2724 nArX	number of X on aromatic ring	Functional group counts
2725 nCXr	number of X on ring C(sp3)	Functional group counts
2726 nCXr=	number of X on ring C(sp2)	Functional group counts
2727 nCconjX	number of X on exo-conjugated C	Functional group counts
2728 nAziridines	number of Aziridines	Functional group counts
2729 nOxiranes	number of Oxiranes	Functional group counts
2730 nThiranes	number of Thiranes	Functional group counts
2731 nAzetidines	number of Azetidines	Functional group counts
2732 nOxetanes	number of Oxetanes	Functional group counts
2733 nThioethanes	number of Thioethanes	Functional group counts
2734 nBeta-Lactams	number of Beta-Lactams	Functional group counts
2735 nPyrrolidines	number of Pyrrolidines	Functional group counts
2736 nOxolanes	number of Oxolanes	Functional group counts
2737 nH-Thiophenes	number of tetrahydro-thiophenes	Functional group counts
2738 nPyrroles	number of Pyrroles	Functional group counts
2739 nPyrazoles	number of Pyrazoles	Functional group counts
2740 nImidazoles	number of Imidazoles	Functional group counts
2741 nFuranes	number of Furanes	Functional group counts
2742 nThiophenes	number of Thiophenes	Functional group counts
2743 nOxazoles	number of Oxazoles	Functional group counts
2744 nIsoxazoles	number of Isoxazoles	Functional group counts
2745 nThiazoles	number of Thiazoles	Functional group counts
2746 nIsothiazoles	number of Isothiazoles	Functional group counts
2747 nTriazoles	number of Triazoles	Functional group counts
2748 nPyridines	number of Pyridines	Functional group counts
2749 nPyridazines	number of Pyridazines	Functional group counts
2750 nPyrimidines	number of Pyrimidines	Functional group counts
2751 nPyrazines	number of Pyrazines	Functional group counts
2752 n135-Triazines	number of 1-3-5-Triazines	Functional group counts
2753 n124-Triazines	number of 1-2-4-Triazines	Functional group counts
2754 nHDon	number of donor atoms for H-bonds (N and O)	Functional group counts
2755 nHAcc	number of acceptor atoms for H-bonds (N,O,F)	Functional group counts
2756 nHBonds	number of intramolecular H-bonds (with N,O,F)	Functional group counts
2757 C-001	CH3R / CH4	Atom-centred fragments
2758 C-002	CH2R2	Atom-centred fragments
2759 C-003	CHR3	Atom-centred fragments
2760 C-004	CR4	Atom-centred fragments
2761 C-005	CH3X	Atom-centred fragments
2762 C-006	CH2RX	Atom-centred fragments
2763 C-007	CH2X2	Atom-centred fragments
2764 C-008	CHR2X	Atom-centred fragments
2765 C-009	CHRX2	Atom-centred fragments
2766 C-010	CHX3	Atom-centred fragments
2767 C-011	CR3X	Atom-centred fragments
2768 C-012	CR2X2	Atom-centred fragments
2769 C-013	CRX3	Atom-centred fragments
2770 C-014	CX4	Atom-centred fragments
2771 C-015	=CH2	Atom-centred fragments
2772 C-016	=CHR	Atom-centred fragments
2773 C-017	=CR2	Atom-centred fragments
2774 C-018	=CHX	Atom-centred fragments
2775 C-019	=CRX	Atom-centred fragments
2776 C-020	=CX2	Atom-centred fragments
2777 C-021	#CH	Atom-centred fragments
2778 C-022	#CR / R=C=R	Atom-centred fragments
2779 C-023	#CX	Atom-centred fragments
2780 C-024	R--CH--R	Atom-centred fragments

2781 C-025	R--CR--R	Atom-centred fragments
2782 C-026	R--CX--R	Atom-centred fragments
2783 C-027	R--CH--X	Atom-centred fragments
2784 C-028	R--CR--X	Atom-centred fragments
2785 C-029	R--CX--X	Atom-centred fragments
2786 C-030	X--CH--X	Atom-centred fragments
2787 C-031	X--CR--X	Atom-centred fragments
2788 C-032	X--CX--X	Atom-centred fragments
2789 C-033	R--CH..X	Atom-centred fragments
2790 C-034	R--CR..X	Atom-centred fragments
2791 C-035	R--CX..X	Atom-centred fragments
2792 C-036	Al-CH=X	Atom-centred fragments
2793 C-037	Ar-CH=X	Atom-centred fragments
2794 C-038	Al-C(=X)-Al	Atom-centred fragments
2795 C-039	Ar-C(=X)-R	Atom-centred fragments
2796 C-040	R-C(=X)-X / R-C#X / X=C=X	Atom-centred fragments
2797 C-041	X-C(=X)-X	Atom-centred fragments
2798 C-042	X--CH..X	Atom-centred fragments
2799 C-043	X--CR..X	Atom-centred fragments
2800 C-044	X--CX..X	Atom-centred fragments
2801 H-046	H attached to C0(sp3) no X attached to next C	Atom-centred fragments
2802 H-047	H attached to C1(sp3)/C0(sp2)	Atom-centred fragments
2803 H-048	H attached to C2(sp3)/C1(sp2)/C0(sp)	Atom-centred fragments
2804 H-049	H attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)	Atom-centred fragments
2805 H-050	H attached to heteroatom	Atom-centred fragments
2806 H-051	H attached to alpha-C	Atom-centred fragments
2807 H-052	H attached to C0(sp3) with 1X attached to next C	Atom-centred fragments
2808 H-053	H attached to C0(sp3) with 2X attached to next C	Atom-centred fragments
2809 H-054	H attached to C0(sp3) with 3X attached to next C	Atom-centred fragments
2810 H-055	H attached to C0(sp3) with 4X attached to next C	Atom-centred fragments
2811 O-056	alcohol	Atom-centred fragments
2812 O-057	phenol / enol / carboxyl OH	Atom-centred fragments
2813 O-058	#NOME?	Atom-centred fragments
2814 O-059	Al-O-Al	Atom-centred fragments
2815 O-060	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X	Atom-centred fragments
2816 O-061	O--	Atom-centred fragments
2817 O-062	O- (negatively charged)	Atom-centred fragments
2818 O-063	R-O-O-R	Atom-centred fragments
2819 Se-064	Any-Se-Any	Atom-centred fragments
2820 Se-065	#NOME?	Atom-centred fragments
2821 N-066	Al-NH2	Atom-centred fragments
2822 N-067	Al2-NH	Atom-centred fragments
2823 N-068	Al3-N	Atom-centred fragments
2824 N-069	Ar-NH2 / X-NH2	Atom-centred fragments
2825 N-070	Ar-NH-Al	Atom-centred fragments
2826 N-071	Ar-NAI2	Atom-centred fragments
2827 N-072	RCO-N< / >N-X=X	Atom-centred fragments
2828 N-073	Ar2NH / Ar3N / Ar2N-Al / R..N..R	Atom-centred fragments
2829 N-074	R#N / R=N-	Atom-centred fragments
2830 N-075	R--N--R / R--N--X	Atom-centred fragments
2831 N-076	Ar-NO2 / R--N(--R)--O / RO-NO	Atom-centred fragments
2832 N-077	Al-NO2	Atom-centred fragments
2833 N-078	Ar-N=X / X-N=X	Atom-centred fragments
2834 N-079	N+ (positively charged)	Atom-centred fragments
2835 F-081	F attached to C1(sp3)	Atom-centred fragments
2836 F-082	F attached to C2(sp3)	Atom-centred fragments
2837 F-083	F attached to C3(sp3)	Atom-centred fragments
2838 F-084	F attached to C1(sp2)	Atom-centred fragments
2839 F-085	F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2840 Cl-086	Cl attached to C1(sp3)	Atom-centred fragments
2841 Cl-087	Cl attached to C2(sp3)	Atom-centred fragments
2842 Cl-088	Cl attached to C3(sp3)	Atom-centred fragments
2843 Cl-089	Cl attached to C1(sp2)	Atom-centred fragments
2844 Cl-090	Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2845 Br-091	Br attached to C1(sp3)	Atom-centred fragments
2846 Br-092	Br attached to C2(sp3)	Atom-centred fragments
2847 Br-093	Br attached to C3(sp3)	Atom-centred fragments
2848 Br-094	Br attached to C1(sp2)	Atom-centred fragments
2849 Br-095	Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2850 I-096	I attached to C1(sp3)	Atom-centred fragments
2851 I-097	I attached to C2(sp3)	Atom-centred fragments
2852 I-098	I attached to C3(sp3)	Atom-centred fragments
2853 I-099	I attached to C1(sp2)	Atom-centred fragments
2854 I-100	I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2855 F-101	fluoride ion	Atom-centred fragments
2856 Cl-102	chloride ion	Atom-centred fragments
2857 Br-103	bromide ion	Atom-centred fragments
2858 I-104	iodide ion	Atom-centred fragments
2859 S-106	R-SH	Atom-centred fragments
2860 S-107	R2S / RS-SR	Atom-centred fragments
2861 S-108	R=S	Atom-centred fragments
2862 S-109	R-SO-R	Atom-centred fragments
2863 S-110	R-SO2-R	Atom-centred fragments
2864 Si-111	>Si<	Atom-centred fragments
2865 B-112	>B- as in boranes	Atom-centred fragments
2866 P-115	P ylids	Atom-centred fragments
2867 P-116	R3-P=X	Atom-centred fragments
2868 P-117	X3-P=X (phosphate)	Atom-centred fragments
2869 P-118	PX3 (phosphite)	Atom-centred fragments
2870 P-119	PR3 (phosphine)	Atom-centred fragments
2871 P-120	C-P(X)2=X (phosphonate)	Atom-centred fragments
2872 SsCH3	Sum of sCH3 E-states	Atom-type E-state indices
2873 SdCH2	Sum of dCH2 E-states	Atom-type E-state indices
2874 SssCH2	Sum of ssCH2 E-states	Atom-type E-state indices
2875 SiCH	Sum of iCH E-states	Atom-type E-state indices
2876 SdsCH	Sum of dsCH E-states	Atom-type E-state indices

2877	SaaCH	Sum of aaCH E-states	Atom-type E-state indices
2878	SsssCH	Sum of ssssCH E-states	Atom-type E-state indices
2879	SddC	Sum of ddC E-states	Atom-type E-state indices
2880	StsC	Sum of tsC E-states	Atom-type E-state indices
2881	SdssC	Sum of dssC E-states	Atom-type E-state indices
2882	SaaC	Sum of aaC E-states	Atom-type E-state indices
2883	SaaaC	Sum of aaaC E-states	Atom-type E-state indices
2884	SssssC	Sum of ssssC E-states	Atom-type E-state indices
2885	SsNH2	Sum of sNH2 E-states	Atom-type E-state indices
2886	SssNH	Sum of ssNH E-states	Atom-type E-state indices
2887	SdNH	Sum of dNH E-states	Atom-type E-state indices
2888	SsssN	Sum of sssN E-states	Atom-type E-state indices
2889	SdsN	Sum of dsN E-states	Atom-type E-state indices
2890	SaaN	Sum of aaN E-states	Atom-type E-state indices
2891	StN	Sum of tN E-states	Atom-type E-state indices
2892	SsNH3+	Sum of sNH3+ E-states	Atom-type E-state indices
2893	SssNH2+	Sum of ssNH2+ E-states	Atom-type E-state indices
2894	SdNH2+	Sum of dNH2+ E-states	Atom-type E-state indices
2895	SsssNH+	Sum of sssNH+ E-states	Atom-type E-state indices
2896	SssssN+	Sum of sssssN+ E-states	Atom-type E-state indices
2897	SddsN	Sum of ddsN E-states	Atom-type E-state indices
2898	SaaN	Sum of aaN E-states	Atom-type E-state indices
2899	SaaNH	Sum of aaNH E-states	Atom-type E-state indices
2900	SsOH	Sum of sOH E-states	Atom-type E-state indices
2901	SdO	Sum of dO E-states	Atom-type E-state indices
2902	SsO	Sum of ssO E-states	Atom-type E-state indices
2903	SaaO	Sum of aaO E-states	Atom-type E-state indices
2904	SsPH2	Sum of sPH2 E-states	Atom-type E-state indices
2905	SssPH	Sum of ssPH E-states	Atom-type E-state indices
2906	SsssP	Sum of sssP E-states	Atom-type E-state indices
2907	SdsssP	Sum of dsssP E-states	Atom-type E-state indices
2908	SddsP	Sum of ddsP E-states	Atom-type E-state indices
2909	SsssssP	Sum of sssssP E-states	Atom-type E-state indices
2910	SsSH	Sum of sSH E-states	Atom-type E-state indices
2911	SdS	Sum of dS E-states	Atom-type E-state indices
2912	SsS	Sum of ssS E-states	Atom-type E-state indices
2913	SaaS	Sum of aaS E-states	Atom-type E-state indices
2914	SdssS	Sum of dssS E-states	Atom-type E-state indices
2915	SddssS	Sum of ddssS E-states	Atom-type E-state indices
2916	SsssssS	Sum of ssssssS E-states	Atom-type E-state indices
2917	SsF	Sum of sF E-states	Atom-type E-state indices
2918	SsCl	Sum of sCl E-states	Atom-type E-state indices
2919	SsBr	Sum of sBr E-states	Atom-type E-state indices
2920	SsI	Sum of sI E-states	Atom-type E-state indices
2921	SsLi	Sum of sLi E-states	Atom-type E-state indices
2922	SsBe	Sum of sBe E-states	Atom-type E-state indices
2923	SssssBe-	Sum of sssssBe- E-states	Atom-type E-state indices
2924	SsBH2	Sum of sBH2 E-states	Atom-type E-state indices
2925	SssBH	Sum of ssBH E-states	Atom-type E-state indices
2926	SsssB	Sum of sssB E-states	Atom-type E-state indices
2927	SssssB-	Sum of sssssB- E-states	Atom-type E-state indices
2928	SsGeH3	Sum of sGeH3 E-states	Atom-type E-state indices
2929	SssGeH2	Sum of ssGeH2 E-states	Atom-type E-state indices
2930	SsssGeH	Sum of sssGeH E-states	Atom-type E-state indices
2931	SssssGe	Sum of sssssGe E-states	Atom-type E-state indices
2932	SsAsH2	Sum of sAsH2 E-states	Atom-type E-state indices
2933	SssAsH	Sum of ssAsH E-states	Atom-type E-state indices
2934	SsssAs	Sum of sssAs E-states	Atom-type E-state indices
2935	SsssssAs	Sum of ssssssAs E-states	Atom-type E-state indices
2936	SdsssAs	Sum of dsssAs E-states	Atom-type E-state indices
2937	SddsAs	Sum of ddsAs E-states	Atom-type E-state indices
2938	SsSeH	Sum of sSeH E-states	Atom-type E-state indices
2939	SdSe	Sum of dSe E-states	Atom-type E-state indices
2940	SssSe	Sum of ssSe E-states	Atom-type E-state indices
2941	SaaSe	Sum of aaSe E-states	Atom-type E-state indices
2942	SdssSe	Sum of dssSe E-states	Atom-type E-state indices
2943	SsssssSe	Sum of ssssssSe E-states	Atom-type E-state indices
2944	SddssSe	Sum of ddssSe E-states	Atom-type E-state indices
2945	SsSnH3	Sum of sSnH3 E-states	Atom-type E-state indices
2946	SssSnH2	Sum of ssSnH2 E-states	Atom-type E-state indices
2947	SsssSnH	Sum of sssSnH E-states	Atom-type E-state indices
2948	SssssSn	Sum of sssssSn E-states	Atom-type E-state indices
2949	SsPbH3	Sum of sPbH3 E-states	Atom-type E-state indices
2950	SssPbH2	Sum of ssPbH2 E-states	Atom-type E-state indices
2951	SsssPbH	Sum of sssPbH E-states	Atom-type E-state indices
2952	SssssPb	Sum of sssssPb E-states	Atom-type E-state indices
2953	SsSiH3	Sum of sSiH3 E-states	Atom-type E-state indices
2954	SssSiH2	Sum of ssSiH2 E-states	Atom-type E-state indices
2955	SsssSiH	Sum of sssSiH E-states	Atom-type E-state indices
2956	SssssSi	Sum of sssssSi E-states	Atom-type E-state indices
2957	NsCH3	Number of atoms of type sCH3	Atom-type E-state indices
2958	NdCH2	Number of atoms of type dCH2	Atom-type E-state indices
2959	NssCH2	Number of atoms of type ssCH2	Atom-type E-state indices
2960	NtCH	Number of atoms of type tCH	Atom-type E-state indices
2961	NdsCH	Number of atoms of type dsCH	Atom-type E-state indices
2962	NaaCH	Number of atoms of type aaCH	Atom-type E-state indices
2963	NsssCH	Number of atoms of type sssCH	Atom-type E-state indices
2964	NddC	Number of atoms of type ddC	Atom-type E-state indices
2965	NtsC	Number of atoms of type tsC	Atom-type E-state indices
2966	NdssC	Number of atoms of type dssC	Atom-type E-state indices
2967	NaasC	Number of atoms of type aaC	Atom-type E-state indices
2968	NaaaC	Number of atoms of type aaaC	Atom-type E-state indices
2969	NssssC	Number of atoms of type ssssC	Atom-type E-state indices
2970	NsNH2	Number of atoms of type sNH2	Atom-type E-state indices
2971	NssNH	Number of atoms of type ssNH	Atom-type E-state indices
2972	NdNH	Number of atoms of type dNH	Atom-type E-state indices

2973	NsssN	Number of atoms of type sssN	Atom-type E-state indices
2974	NdsN	Number of atoms of type dsN	Atom-type E-state indices
2975	NaaN	Number of atoms of type aaN	Atom-type E-state indices
2976	NIN	Number of atoms of type tN	Atom-type E-state indices
2977	NsNH3+	Number of atoms of type sNH3+	Atom-type E-state indices
2978	NssNH2+	Number of atoms of type ssNH2+	Atom-type E-state indices
2979	NdNH2+	Number of atoms of type dNH2+	Atom-type E-state indices
2980	NsssNH+	Number of atoms of type sssNH+	Atom-type E-state indices
2981	NssssN+	Number of atoms of type sssssN+	Atom-type E-state indices
2982	NddsN	Number of atoms of type ddsN	Atom-type E-state indices
2983	NaasN	Number of atoms of type aasN	Atom-type E-state indices
2984	NaaNH	Number of atoms of type aaNH	Atom-type E-state indices
2985	NsOH	Number of atoms of type sOH	Atom-type E-state indices
2986	NdO	Number of atoms of type dO	Atom-type E-state indices
2987	NssO	Number of atoms of type ssO	Atom-type E-state indices
2988	NaaO	Number of atoms of type aaO	Atom-type E-state indices
2989	NsPH2	Number of atoms of type sPH2	Atom-type E-state indices
2990	NssPH	Number of atoms of type ssPH	Atom-type E-state indices
2991	NssSP	Number of atoms of type sssP	Atom-type E-state indices
2992	NdsssP	Number of atoms of type dsssP	Atom-type E-state indices
2993	NddSP	Number of atoms of type ddsP	Atom-type E-state indices
2994	NsssssP	Number of atoms of type sssssP	Atom-type E-state indices
2995	NsSH	Number of atoms of type sSH	Atom-type E-state indices
2996	NdS	Number of atoms of type dS	Atom-type E-state indices
2997	NssS	Number of atoms of type ssS	Atom-type E-state indices
2998	NaaS	Number of atoms of type aaS	Atom-type E-state indices
2999	NdssS	Number of atoms of type dssS	Atom-type E-state indices
3000	NddssS	Number of atoms of type ddsS	Atom-type E-state indices
3001	NssssssS	Number of atoms of type ssssssS	Atom-type E-state indices
3002	NsF	Number of atoms of type sF	Atom-type E-state indices
3003	NsCl	Number of atoms of type sCl	Atom-type E-state indices
3004	NsBr	Number of atoms of type sBr	Atom-type E-state indices
3005	NsI	Number of atoms of type sI	Atom-type E-state indices
3006	NsLi	Number of atoms of type sLi	Atom-type E-state indices
3007	NssBe	Number of atoms of type ssBe	Atom-type E-state indices
3008	NssssBe-	Number of atoms of type sssssBe-	Atom-type E-state indices
3009	NsBH2	Number of atoms of type sBH2	Atom-type E-state indices
3010	NssBH	Number of atoms of type ssBH	Atom-type E-state indices
3011	NssSB	Number of atoms of type sssB	Atom-type E-state indices
3012	NssssB-	Number of atoms of type sssssB-	Atom-type E-state indices
3013	NsGeH3	Number of atoms of type sGeH3	Atom-type E-state indices
3014	NssGeH2	Number of atoms of type ssGeH2	Atom-type E-state indices
3015	NssssGeH	Number of atoms of type sssGeH	Atom-type E-state indices
3016	NssssGe	Number of atoms of type sssssGe	Atom-type E-state indices
3017	NsAsH2	Number of atoms of type sAsH2	Atom-type E-state indices
3018	NssAsH	Number of atoms of type ssAsH	Atom-type E-state indices
3019	NssAs	Number of atoms of type sssAs	Atom-type E-state indices
3020	NsssssAs	Number of atoms of type ssssssAs	Atom-type E-state indices
3021	NdsssAs	Number of atoms of type dsssAs	Atom-type E-state indices
3022	NddsAs	Number of atoms of type ddsAs	Atom-type E-state indices
3023	NsSeH	Number of atoms of type sSeH	Atom-type E-state indices
3024	NdSe	Number of atoms of type dSe	Atom-type E-state indices
3025	NssSe	Number of atoms of type ssSe	Atom-type E-state indices
3026	NaaSe	Number of atoms of type aaSe	Atom-type E-state indices
3027	NdssSe	Number of atoms of type dssSe	Atom-type E-state indices
3028	NssssssSe	Number of atoms of type ssssssSe	Atom-type E-state indices
3029	NddssSe	Number of atoms of type ddsSe	Atom-type E-state indices
3030	NsSnH3	Number of atoms of type sSnH3	Atom-type E-state indices
3031	NssSnH2	Number of atoms of type ssSnH2	Atom-type E-state indices
3032	NssSnH	Number of atoms of type sssSnH	Atom-type E-state indices
3033	NssssSn	Number of atoms of type sssssSn	Atom-type E-state indices
3034	NsPbH3	Number of atoms of type sPbH3	Atom-type E-state indices
3035	NssPbH2	Number of atoms of type ssPbH2	Atom-type E-state indices
3036	NssPbH	Number of atoms of type sssPbH	Atom-type E-state indices
3037	NssssPb	Number of atoms of type sssssPb	Atom-type E-state indices
3038	NsSiH3	Number of atoms of type sSiH3	Atom-type E-state indices
3039	NssSiH2	Number of atoms of type ssSiH2	Atom-type E-state indices
3040	NssSiH	Number of atoms of type sssSiH	Atom-type E-state indices
3041	NssSi	Number of atoms of type sssSi	Atom-type E-state indices
3042	CATS2D_00_DD	CATS2D Donor-Donor at lag 00	CATS 2D
3043	CATS2D_01_DD	CATS2D Donor-Donor at lag 01	CATS 2D
3044	CATS2D_02_DD	CATS2D Donor-Donor at lag 02	CATS 2D
3045	CATS2D_03_DD	CATS2D Donor-Donor at lag 03	CATS 2D
3046	CATS2D_04_DD	CATS2D Donor-Donor at lag 04	CATS 2D
3047	CATS2D_05_DD	CATS2D Donor-Donor at lag 05	CATS 2D
3048	CATS2D_06_DD	CATS2D Donor-Donor at lag 06	CATS 2D
3049	CATS2D_07_DD	CATS2D Donor-Donor at lag 07	CATS 2D
3050	CATS2D_08_DD	CATS2D Donor-Donor at lag 08	CATS 2D
3051	CATS2D_09_DD	CATS2D Donor-Donor at lag 09	CATS 2D
3052	CATS2D_00_DA	CATS2D Donor-Acceptor at lag 00	CATS 2D
3053	CATS2D_01_DA	CATS2D Donor-Acceptor at lag 01	CATS 2D
3054	CATS2D_02_DA	CATS2D Donor-Acceptor at lag 02	CATS 2D
3055	CATS2D_03_DA	CATS2D Donor-Acceptor at lag 03	CATS 2D
3056	CATS2D_04_DA	CATS2D Donor-Acceptor at lag 04	CATS 2D
3057	CATS2D_05_DA	CATS2D Donor-Acceptor at lag 05	CATS 2D
3058	CATS2D_06_DA	CATS2D Donor-Acceptor at lag 06	CATS 2D
3059	CATS2D_07_DA	CATS2D Donor-Acceptor at lag 07	CATS 2D
3060	CATS2D_08_DA	CATS2D Donor-Acceptor at lag 08	CATS 2D
3061	CATS2D_09_DA	CATS2D Donor-Acceptor at lag 09	CATS 2D
3062	CATS2D_00_DP	CATS2D Donor-Positive at lag 00	CATS 2D
3063	CATS2D_01_DP	CATS2D Donor-Positive at lag 01	CATS 2D
3064	CATS2D_02_DP	CATS2D Donor-Positive at lag 02	CATS 2D
3065	CATS2D_03_DP	CATS2D Donor-Positive at lag 03	CATS 2D
3066	CATS2D_04_DP	CATS2D Donor-Positive at lag 04	CATS 2D
3067	CATS2D_05_DP	CATS2D Donor-Positive at lag 05	CATS 2D
3068	CATS2D_06_DP	CATS2D Donor-Positive at lag 06	CATS 2D





3165	CATS2D_03_NN	CATS2D Negative-Negative at lag 03	CATS 2D
3166	CATS2D_04_NN	CATS2D Negative-Negative at lag 04	CATS 2D
3167	CATS2D_05_NN	CATS2D Negative-Negative at lag 05	CATS 2D
3168	CATS2D_06_NN	CATS2D Negative-Negative at lag 06	CATS 2D
3169	CATS2D_07_NN	CATS2D Negative-Negative at lag 07	CATS 2D
3170	CATS2D_08_NN	CATS2D Negative-Negative at lag 08	CATS 2D
3171	CATS2D_09_NN	CATS2D Negative-Negative at lag 09	CATS 2D
3172	CATS2D_00_NL	CATS2D Negative-Lipophilic at lag 00	CATS 2D
3173	CATS2D_01_NL	CATS2D Negative-Lipophilic at lag 01	CATS 2D
3174	CATS2D_02_NL	CATS2D Negative-Lipophilic at lag 02	CATS 2D
3175	CATS2D_03_NL	CATS2D Negative-Lipophilic at lag 03	CATS 2D
3176	CATS2D_04_NL	CATS2D Negative-Lipophilic at lag 04	CATS 2D
3177	CATS2D_05_NL	CATS2D Negative-Lipophilic at lag 05	CATS 2D
3178	CATS2D_06_NL	CATS2D Negative-Lipophilic at lag 06	CATS 2D
3179	CATS2D_07_NL	CATS2D Negative-Lipophilic at lag 07	CATS 2D
3180	CATS2D_08_NL	CATS2D Negative-Lipophilic at lag 08	CATS 2D
3181	CATS2D_09_NL	CATS2D Negative-Lipophilic at lag 09	CATS 2D
3182	CATS2D_00_LL	CATS2D Lipophilic-Lipophilic at lag 00	CATS 2D
3183	CATS2D_01_LL	CATS2D Lipophilic-Lipophilic at lag 01	CATS 2D
3184	CATS2D_02_LL	CATS2D Lipophilic-Lipophilic at lag 02	CATS 2D
3185	CATS2D_03_LL	CATS2D Lipophilic-Lipophilic at lag 03	CATS 2D
3186	CATS2D_04_LL	CATS2D Lipophilic-Lipophilic at lag 04	CATS 2D
3187	CATS2D_05_LL	CATS2D Lipophilic-Lipophilic at lag 05	CATS 2D
3188	CATS2D_06_LL	CATS2D Lipophilic-Lipophilic at lag 06	CATS 2D
3189	CATS2D_07_LL	CATS2D Lipophilic-Lipophilic at lag 07	CATS 2D
3190	CATS2D_08_LL	CATS2D Lipophilic-Lipophilic at lag 08	CATS 2D
3191	CATS2D_09_LL	CATS2D Lipophilic-Lipophilic at lag 09	CATS 2D
3192	T(N..N)	sum of topological distances between N..N	2D Atom Pairs
3193	T(N..O)	sum of topological distances between N..O	2D Atom Pairs
3194	T(N..S)	sum of topological distances between N..S	2D Atom Pairs
3195	T(N..P)	sum of topological distances between N..P	2D Atom Pairs
3196	T(N..F)	sum of topological distances between N..F	2D Atom Pairs
3197	T(N..Cl)	sum of topological distances between N..Cl	2D Atom Pairs
3198	T(N..Br)	sum of topological distances between N..Br	2D Atom Pairs
3199	T(N..I)	sum of topological distances between N..I	2D Atom Pairs
3200	T(O..O)	sum of topological distances between O..O	2D Atom Pairs
3201	T(O..S)	sum of topological distances between O..S	2D Atom Pairs
3202	T(O..P)	sum of topological distances between O..P	2D Atom Pairs
3203	T(O..F)	sum of topological distances between O..F	2D Atom Pairs
3204	T(O..Cl)	sum of topological distances between O..Cl	2D Atom Pairs
3205	T(O..Br)	sum of topological distances between O..Br	2D Atom Pairs
3206	T(O..I)	sum of topological distances between O..I	2D Atom Pairs
3207	T(S..S)	sum of topological distances between S..S	2D Atom Pairs
3208	T(S..P)	sum of topological distances between S..P	2D Atom Pairs
3209	T(S..F)	sum of topological distances between S..F	2D Atom Pairs
3210	T(S..Cl)	sum of topological distances between S..Cl	2D Atom Pairs
3211	T(S..Br)	sum of topological distances between S..Br	2D Atom Pairs
3212	T(S..I)	sum of topological distances between S..I	2D Atom Pairs
3213	T(P..P)	sum of topological distances between P..P	2D Atom Pairs
3214	T(P..F)	sum of topological distances between P..F	2D Atom Pairs
3215	T(P..Cl)	sum of topological distances between P..Cl	2D Atom Pairs
3216	T(P..Br)	sum of topological distances between P..Br	2D Atom Pairs
3217	T(P..I)	sum of topological distances between P..I	2D Atom Pairs
3218	T(F..F)	sum of topological distances between F..F	2D Atom Pairs
3219	T(F..Cl)	sum of topological distances between F..Cl	2D Atom Pairs
3220	T(F..Br)	sum of topological distances between F..Br	2D Atom Pairs
3221	T(F..I)	sum of topological distances between F..I	2D Atom Pairs
3222	T(Cl..Cl)	sum of topological distances between Cl..Cl	2D Atom Pairs
3223	T(Cl..Br)	sum of topological distances between Cl..Br	2D Atom Pairs
3224	T(Cl..I)	sum of topological distances between Cl..I	2D Atom Pairs
3225	T(Br..Br)	sum of topological distances between Br..Br	2D Atom Pairs
3226	T(Br..I)	sum of topological distances between Br..I	2D Atom Pairs
3227	T(I..I)	sum of topological distances between I..I	2D Atom Pairs
3228	B01[C-C]	Presence/absence of C - C at topological distance 1	2D Atom Pairs
3229	B01[C-N]	Presence/absence of C - N at topological distance 1	2D Atom Pairs
3230	B01[C-O]	Presence/absence of C - O at topological distance 1	2D Atom Pairs
3231	B01[C-S]	Presence/absence of C - S at topological distance 1	2D Atom Pairs
3232	B01[C-P]	Presence/absence of C - P at topological distance 1	2D Atom Pairs
3233	B01[C-F]	Presence/absence of C - F at topological distance 1	2D Atom Pairs
3234	B01[C-Cl]	Presence/absence of C - Cl at topological distance 1	2D Atom Pairs
3235	B01[C-Br]	Presence/absence of C - Br at topological distance 1	2D Atom Pairs
3236	B01[C-I]	Presence/absence of C - I at topological distance 1	2D Atom Pairs
3237	B01[C-B]	Presence/absence of C - B at topological distance 1	2D Atom Pairs
3238	B01[C-Si]	Presence/absence of C - Si at topological distance 1	2D Atom Pairs
3239	B01[C-X]	Presence/absence of C - X at topological distance 1	2D Atom Pairs
3240	B01[N-N]	Presence/absence of N - N at topological distance 1	2D Atom Pairs
3241	B01[N-O]	Presence/absence of N - O at topological distance 1	2D Atom Pairs
3242	B01[N-S]	Presence/absence of N - S at topological distance 1	2D Atom Pairs
3243	B01[N-P]	Presence/absence of N - P at topological distance 1	2D Atom Pairs
3244	B01[N-F]	Presence/absence of N - F at topological distance 1	2D Atom Pairs
3245	B01[N-Cl]	Presence/absence of N - Cl at topological distance 1	2D Atom Pairs
3246	B01[N-Br]	Presence/absence of N - Br at topological distance 1	2D Atom Pairs
3247	B01[N-I]	Presence/absence of N - I at topological distance 1	2D Atom Pairs
3248	B01[N-B]	Presence/absence of N - B at topological distance 1	2D Atom Pairs
3249	B01[N-Si]	Presence/absence of N - Si at topological distance 1	2D Atom Pairs
3250	B01[N-X]	Presence/absence of N - X at topological distance 1	2D Atom Pairs
3251	B01[O-O]	Presence/absence of O - O at topological distance 1	2D Atom Pairs
3252	B01[O-S]	Presence/absence of O - S at topological distance 1	2D Atom Pairs
3253	B01[O-P]	Presence/absence of O - P at topological distance 1	2D Atom Pairs
3254	B01[O-F]	Presence/absence of O - F at topological distance 1	2D Atom Pairs
3255	B01[O-Cl]	Presence/absence of O - Cl at topological distance 1	2D Atom Pairs
3256	B01[O-Br]	Presence/absence of O - Br at topological distance 1	2D Atom Pairs
3257	B01[O-I]	Presence/absence of O - I at topological distance 1	2D Atom Pairs
3258	B01[O-B]	Presence/absence of O - B at topological distance 1	2D Atom Pairs
3259	B01[O-Si]	Presence/absence of O - Si at topological distance 1	2D Atom Pairs
3260	B01[O-X]	Presence/absence of O - X at topological distance 1	2D Atom Pairs





































4605	F08[F-C]	Frequency of F - Cl at topological distance 8	2D Atom Pairs
4606	F08[F-Br]	Frequency of F - Br at topological distance 8	2D Atom Pairs
4607	F08[F-I]	Frequency of F - I at topological distance 8	2D Atom Pairs
4608	F08[F-B]	Frequency of F - B at topological distance 8	2D Atom Pairs
4609	F08[F-Si]	Frequency of F - Si at topological distance 8	2D Atom Pairs
4610	F08[F-X]	Frequency of F - X at topological distance 8	2D Atom Pairs
4611	F08[Cl-Cl]	Frequency of Cl - Cl at topological distance 8	2D Atom Pairs
4612	F08[Cl-Br]	Frequency of Cl - Br at topological distance 8	2D Atom Pairs
4613	F08[Cl-I]	Frequency of Cl - I at topological distance 8	2D Atom Pairs
4614	F08[Cl-B]	Frequency of Cl - B at topological distance 8	2D Atom Pairs
4615	F08[Cl-Si]	Frequency of Cl - Si at topological distance 8	2D Atom Pairs
4616	F08[Cl-X]	Frequency of Cl - X at topological distance 8	2D Atom Pairs
4617	F08[Br-Br]	Frequency of Br - Br at topological distance 8	2D Atom Pairs
4618	F08[Br-I]	Frequency of Br - I at topological distance 8	2D Atom Pairs
4619	F08[Br-B]	Frequency of Br - B at topological distance 8	2D Atom Pairs
4620	F08[Br-Si]	Frequency of Br - Si at topological distance 8	2D Atom Pairs
4621	F08[Br-X]	Frequency of Br - X at topological distance 8	2D Atom Pairs
4622	F08[I-I]	Frequency of I - I at topological distance 8	2D Atom Pairs
4623	F08[I-B]	Frequency of I - B at topological distance 8	2D Atom Pairs
4624	F08[I-Si]	Frequency of I - Si at topological distance 8	2D Atom Pairs
4625	F08[I-X]	Frequency of I - X at topological distance 8	2D Atom Pairs
4626	F08[B-B]	Frequency of B - B at topological distance 8	2D Atom Pairs
4627	F08[B-Si]	Frequency of B - Si at topological distance 8	2D Atom Pairs
4628	F08[B-X]	Frequency of B - X at topological distance 8	2D Atom Pairs
4629	F08[Si-Si]	Frequency of Si - Si at topological distance 8	2D Atom Pairs
4630	F08[Si-X]	Frequency of Si - X at topological distance 8	2D Atom Pairs
4631	F08[X-X]	Frequency of X - X at topological distance 8	2D Atom Pairs
4632	F09[C-C]	Frequency of C - C at topological distance 9	2D Atom Pairs
4633	F09[C-N]	Frequency of C - N at topological distance 9	2D Atom Pairs
4634	F09[C-O]	Frequency of C - O at topological distance 9	2D Atom Pairs
4635	F09[C-S]	Frequency of C - S at topological distance 9	2D Atom Pairs
4636	F09[C-P]	Frequency of C - P at topological distance 9	2D Atom Pairs
4637	F09[C-F]	Frequency of C - F at topological distance 9	2D Atom Pairs
4638	F09[C-Cl]	Frequency of C - Cl at topological distance 9	2D Atom Pairs
4639	F09[C-Br]	Frequency of C - Br at topological distance 9	2D Atom Pairs
4640	F09[C-I]	Frequency of C - I at topological distance 9	2D Atom Pairs
4641	F09[C-B]	Frequency of C - B at topological distance 9	2D Atom Pairs
4642	F09[C-Si]	Frequency of C - Si at topological distance 9	2D Atom Pairs
4643	F09[C-X]	Frequency of C - X at topological distance 9	2D Atom Pairs
4644	F09[N-N]	Frequency of N - N at topological distance 9	2D Atom Pairs
4645	F09[N-O]	Frequency of N - O at topological distance 9	2D Atom Pairs
4646	F09[N-S]	Frequency of N - S at topological distance 9	2D Atom Pairs
4647	F09[N-P]	Frequency of N - P at topological distance 9	2D Atom Pairs
4648	F09[N-F]	Frequency of N - F at topological distance 9	2D Atom Pairs
4649	F09[N-Cl]	Frequency of N - Cl at topological distance 9	2D Atom Pairs
4650	F09[N-Br]	Frequency of N - Br at topological distance 9	2D Atom Pairs
4651	F09[N-I]	Frequency of N - I at topological distance 9	2D Atom Pairs
4652	F09[N-B]	Frequency of N - B at topological distance 9	2D Atom Pairs
4653	F09[N-Si]	Frequency of N - Si at topological distance 9	2D Atom Pairs
4654	F09[N-X]	Frequency of N - X at topological distance 9	2D Atom Pairs
4655	F09[O-O]	Frequency of O - O at topological distance 9	2D Atom Pairs
4656	F09[O-S]	Frequency of O - S at topological distance 9	2D Atom Pairs
4657	F09[O-P]	Frequency of O - P at topological distance 9	2D Atom Pairs
4658	F09[O-F]	Frequency of O - F at topological distance 9	2D Atom Pairs
4659	F09[O-Cl]	Frequency of O - Cl at topological distance 9	2D Atom Pairs
4660	F09[O-Br]	Frequency of O - Br at topological distance 9	2D Atom Pairs
4661	F09[O-I]	Frequency of O - I at topological distance 9	2D Atom Pairs
4662	F09[O-B]	Frequency of O - B at topological distance 9	2D Atom Pairs
4663	F09[O-Si]	Frequency of O - Si at topological distance 9	2D Atom Pairs
4664	F09[O-X]	Frequency of O - X at topological distance 9	2D Atom Pairs
4665	F09[S-S]	Frequency of S - S at topological distance 9	2D Atom Pairs
4666	F09[S-P]	Frequency of S - P at topological distance 9	2D Atom Pairs
4667	F09[S-F]	Frequency of S - F at topological distance 9	2D Atom Pairs
4668	F09[S-Cl]	Frequency of S - Cl at topological distance 9	2D Atom Pairs
4669	F09[S-Br]	Frequency of S - Br at topological distance 9	2D Atom Pairs
4670	F09[S-I]	Frequency of S - I at topological distance 9	2D Atom Pairs
4671	F09[S-B]	Frequency of S - B at topological distance 9	2D Atom Pairs
4672	F09[S-Si]	Frequency of S - Si at topological distance 9	2D Atom Pairs
4673	F09[S-X]	Frequency of S - X at topological distance 9	2D Atom Pairs
4674	F09[P-P]	Frequency of P - P at topological distance 9	2D Atom Pairs
4675	F09[P-F]	Frequency of P - F at topological distance 9	2D Atom Pairs
4676	F09[P-Cl]	Frequency of P - Cl at topological distance 9	2D Atom Pairs
4677	F09[P-Br]	Frequency of P - Br at topological distance 9	2D Atom Pairs
4678	F09[P-I]	Frequency of P - I at topological distance 9	2D Atom Pairs
4679	F09[P-B]	Frequency of P - B at topological distance 9	2D Atom Pairs
4680	F09[P-Si]	Frequency of P - Si at topological distance 9	2D Atom Pairs
4681	F09[P-X]	Frequency of P - X at topological distance 9	2D Atom Pairs
4682	F09[F-F]	Frequency of F - F at topological distance 9	2D Atom Pairs
4683	F09[F-Cl]	Frequency of F - Cl at topological distance 9	2D Atom Pairs
4684	F09[F-Br]	Frequency of F - Br at topological distance 9	2D Atom Pairs
4685	F09[F-I]	Frequency of F - I at topological distance 9	2D Atom Pairs
4686	F09[F-B]	Frequency of F - B at topological distance 9	2D Atom Pairs
4687	F09[F-Si]	Frequency of F - Si at topological distance 9	2D Atom Pairs
4688	F09[F-X]	Frequency of F - X at topological distance 9	2D Atom Pairs
4689	F09[Cl-Cl]	Frequency of Cl - Cl at topological distance 9	2D Atom Pairs
4690	F09[Cl-Br]	Frequency of Cl - Br at topological distance 9	2D Atom Pairs
4691	F09[Cl-I]	Frequency of Cl - I at topological distance 9	2D Atom Pairs
4692	F09[Cl-B]	Frequency of Cl - B at topological distance 9	2D Atom Pairs
4693	F09[Cl-Si]	Frequency of Cl - Si at topological distance 9	2D Atom Pairs
4694	F09[Cl-X]	Frequency of Cl - X at topological distance 9	2D Atom Pairs
4695	F09[Br-Br]	Frequency of Br - Br at topological distance 9	2D Atom Pairs
4696	F09[Br-I]	Frequency of Br - I at topological distance 9	2D Atom Pairs
4697	F09[Br-B]	Frequency of Br - B at topological distance 9	2D Atom Pairs
4698	F09[Br-Si]	Frequency of Br - Si at topological distance 9	2D Atom Pairs
4699	F09[Br-X]	Frequency of Br - X at topological distance 9	2D Atom Pairs
4700	F09[I-I]	Frequency of I - I at topological distance 9	2D Atom Pairs

4701	F09[I-B]	Frequency of I - B at topological distance 9	2D Atom Pairs
4702	F09[I-Si]	Frequency of I - Si at topological distance 9	2D Atom Pairs
4703	F09[I-X]	Frequency of I - X at topological distance 9	2D Atom Pairs
4704	F09[B-B]	Frequency of B - B at topological distance 9	2D Atom Pairs
4705	F09[B-Si]	Frequency of B - Si at topological distance 9	2D Atom Pairs
4706	F09[B-X]	Frequency of B - X at topological distance 9	2D Atom Pairs
4707	F09[Si-Si]	Frequency of Si - Si at topological distance 9	2D Atom Pairs
4708	F09[Si-X]	Frequency of Si - X at topological distance 9	2D Atom Pairs
4709	F09[X-X]	Frequency of X - X at topological distance 9	2D Atom Pairs
4710	F10[C-C]	Frequency of C - C at topological distance 10	2D Atom Pairs
4711	F10[C-N]	Frequency of C - N at topological distance 10	2D Atom Pairs
4712	F10[C-O]	Frequency of C - O at topological distance 10	2D Atom Pairs
4713	F10[C-S]	Frequency of C - S at topological distance 10	2D Atom Pairs
4714	F10[C-P]	Frequency of C - P at topological distance 10	2D Atom Pairs
4715	F10[C-F]	Frequency of C - F at topological distance 10	2D Atom Pairs
4716	F10[C-Cl]	Frequency of C - Cl at topological distance 10	2D Atom Pairs
4717	F10[C-Br]	Frequency of C - Br at topological distance 10	2D Atom Pairs
4718	F10[C-I]	Frequency of C - I at topological distance 10	2D Atom Pairs
4719	F10[C-B]	Frequency of C - B at topological distance 10	2D Atom Pairs
4720	F10[C-Si]	Frequency of C - Si at topological distance 10	2D Atom Pairs
4721	F10[C-X]	Frequency of C - X at topological distance 10	2D Atom Pairs
4722	F10[N-N]	Frequency of N - N at topological distance 10	2D Atom Pairs
4723	F10[N-O]	Frequency of N - O at topological distance 10	2D Atom Pairs
4724	F10[N-S]	Frequency of N - S at topological distance 10	2D Atom Pairs
4725	F10[N-P]	Frequency of N - P at topological distance 10	2D Atom Pairs
4726	F10[N-F]	Frequency of N - F at topological distance 10	2D Atom Pairs
4727	F10[N-Cl]	Frequency of N - Cl at topological distance 10	2D Atom Pairs
4728	F10[N-Br]	Frequency of N - Br at topological distance 10	2D Atom Pairs
4729	F10[N-I]	Frequency of N - I at topological distance 10	2D Atom Pairs
4730	F10[N-B]	Frequency of N - B at topological distance 10	2D Atom Pairs
4731	F10[N-Si]	Frequency of N - Si at topological distance 10	2D Atom Pairs
4732	F10[N-X]	Frequency of N - X at topological distance 10	2D Atom Pairs
4733	F10[O-O]	Frequency of O - O at topological distance 10	2D Atom Pairs
4734	F10[O-S]	Frequency of O - S at topological distance 10	2D Atom Pairs
4735	F10[O-P]	Frequency of O - P at topological distance 10	2D Atom Pairs
4736	F10[O-F]	Frequency of O - F at topological distance 10	2D Atom Pairs
4737	F10[O-Cl]	Frequency of O - Cl at topological distance 10	2D Atom Pairs
4738	F10[O-Br]	Frequency of O - Br at topological distance 10	2D Atom Pairs
4739	F10[O-I]	Frequency of O - I at topological distance 10	2D Atom Pairs
4740	F10[O-B]	Frequency of O - B at topological distance 10	2D Atom Pairs
4741	F10[O-Si]	Frequency of O - Si at topological distance 10	2D Atom Pairs
4742	F10[O-X]	Frequency of O - X at topological distance 10	2D Atom Pairs
4743	F10[S-S]	Frequency of S - S at topological distance 10	2D Atom Pairs
4744	F10[S-P]	Frequency of S - P at topological distance 10	2D Atom Pairs
4745	F10[S-F]	Frequency of S - F at topological distance 10	2D Atom Pairs
4746	F10[S-Cl]	Frequency of S - Cl at topological distance 10	2D Atom Pairs
4747	F10[S-Br]	Frequency of S - Br at topological distance 10	2D Atom Pairs
4748	F10[S-I]	Frequency of S - I at topological distance 10	2D Atom Pairs
4749	F10[S-B]	Frequency of S - B at topological distance 10	2D Atom Pairs
4750	F10[S-Si]	Frequency of S - Si at topological distance 10	2D Atom Pairs
4751	F10[S-X]	Frequency of S - X at topological distance 10	2D Atom Pairs
4752	F10[P-P]	Frequency of P - P at topological distance 10	2D Atom Pairs
4753	F10[P-F]	Frequency of P - F at topological distance 10	2D Atom Pairs
4754	F10[P-Cl]	Frequency of P - Cl at topological distance 10	2D Atom Pairs
4755	F10[P-Br]	Frequency of P - Br at topological distance 10	2D Atom Pairs
4756	F10[P-I]	Frequency of P - I at topological distance 10	2D Atom Pairs
4757	F10[P-B]	Frequency of P - B at topological distance 10	2D Atom Pairs
4758	F10[P-Si]	Frequency of P - Si at topological distance 10	2D Atom Pairs
4759	F10[P-X]	Frequency of P - X at topological distance 10	2D Atom Pairs
4760	F10[F-F]	Frequency of F - F at topological distance 10	2D Atom Pairs
4761	F10[F-Cl]	Frequency of F - Cl at topological distance 10	2D Atom Pairs
4762	F10[F-Br]	Frequency of F - Br at topological distance 10	2D Atom Pairs
4763	F10[F-I]	Frequency of F - I at topological distance 10	2D Atom Pairs
4764	F10[F-B]	Frequency of F - B at topological distance 10	2D Atom Pairs
4765	F10[F-Si]	Frequency of F - Si at topological distance 10	2D Atom Pairs
4766	F10[F-X]	Frequency of F - X at topological distance 10	2D Atom Pairs
4767	F10[Cl-Cl]	Frequency of Cl - Cl at topological distance 10	2D Atom Pairs
4768	F10[Cl-Br]	Frequency of Cl - Br at topological distance 10	2D Atom Pairs
4769	F10[Cl-I]	Frequency of Cl - I at topological distance 10	2D Atom Pairs
4770	F10[Cl-B]	Frequency of Cl - B at topological distance 10	2D Atom Pairs
4771	F10[Cl-Si]	Frequency of Cl - Si at topological distance 10	2D Atom Pairs
4772	F10[Cl-X]	Frequency of Cl - X at topological distance 10	2D Atom Pairs
4773	F10[Br-Br]	Frequency of Br - Br at topological distance 10	2D Atom Pairs
4774	F10[Br-I]	Frequency of Br - I at topological distance 10	2D Atom Pairs
4775	F10[Br-B]	Frequency of Br - B at topological distance 10	2D Atom Pairs
4776	F10[Br-Si]	Frequency of Br - Si at topological distance 10	2D Atom Pairs
4777	F10[Br-X]	Frequency of Br - X at topological distance 10	2D Atom Pairs
4778	F10[I-I]	Frequency of I - I at topological distance 10	2D Atom Pairs
4779	F10[I-B]	Frequency of I - B at topological distance 10	2D Atom Pairs
4780	F10[I-Si]	Frequency of I - Si at topological distance 10	2D Atom Pairs
4781	F10[I-X]	Frequency of I - X at topological distance 10	2D Atom Pairs
4782	F10[B-B]	Frequency of B - B at topological distance 10	2D Atom Pairs
4783	F10[B-Si]	Frequency of B - Si at topological distance 10	2D Atom Pairs
4784	F10[B-X]	Frequency of B - X at topological distance 10	2D Atom Pairs
4785	F10[Si-Si]	Frequency of Si - Si at topological distance 10	2D Atom Pairs
4786	F10[Si-X]	Frequency of Si - X at topological distance 10	2D Atom Pairs
4787	F10[X-X]	Frequency of X - X at topological distance 10	2D Atom Pairs
4788	G(N..N)	sum of geometrical distances between N..N	3D Atom Pairs
4789	G(N..O)	sum of geometrical distances between N..O	3D Atom Pairs
4790	G(N..S)	sum of geometrical distances between N..S	3D Atom Pairs
4791	G(N..P)	sum of geometrical distances between N..P	3D Atom Pairs
4792	G(N..F)	sum of geometrical distances between N..F	3D Atom Pairs
4793	G(N..Cl)	sum of geometrical distances between N..Cl	3D Atom Pairs
4794	G(N..Br)	sum of geometrical distances between N..Br	3D Atom Pairs
4795	G(N..I)	sum of geometrical distances between N..I	3D Atom Pairs
4796	G(O..O)	sum of geometrical distances between O..O	3D Atom Pairs

4797	G(O..S)	sum of geometrical distances between O..S	3D Atom Pairs
4798	G(O..P)	sum of geometrical distances between O..P	3D Atom Pairs
4799	G(O..F)	sum of geometrical distances between O..F	3D Atom Pairs
4800	G(O..Cl)	sum of geometrical distances between O..Cl	3D Atom Pairs
4801	G(O..Br)	sum of geometrical distances between O..Br	3D Atom Pairs
4802	G(O..I)	sum of geometrical distances between O..I	3D Atom Pairs
4803	G(S..S)	sum of geometrical distances between S..S	3D Atom Pairs
4804	G(S..P)	sum of geometrical distances between S..P	3D Atom Pairs
4805	G(S..F)	sum of geometrical distances between S..F	3D Atom Pairs
4806	G(S..Cl)	sum of geometrical distances between S..Cl	3D Atom Pairs
4807	G(S..Br)	sum of geometrical distances between S..Br	3D Atom Pairs
4808	G(S..I)	sum of geometrical distances between S..I	3D Atom Pairs
4809	G(P..P)	sum of geometrical distances between P..P	3D Atom Pairs
4810	G(P..F)	sum of geometrical distances between P..F	3D Atom Pairs
4811	G(P..Cl)	sum of geometrical distances between P..Cl	3D Atom Pairs
4812	G(P..Br)	sum of geometrical distances between P..Br	3D Atom Pairs
4813	G(P..I)	sum of geometrical distances between P..I	3D Atom Pairs
4814	G(F..F)	sum of geometrical distances between F..F	3D Atom Pairs
4815	G(F..Cl)	sum of geometrical distances between F..Cl	3D Atom Pairs
4816	G(F..Br)	sum of geometrical distances between F..Br	3D Atom Pairs
4817	G(F..I)	sum of geometrical distances between F..I	3D Atom Pairs
4818	G(Cl..Cl)	sum of geometrical distances between Cl..Cl	3D Atom Pairs
4819	G(Cl..Br)	sum of geometrical distances between Cl..Br	3D Atom Pairs
4820	G(Cl..I)	sum of geometrical distances between Cl..I	3D Atom Pairs
4821	G(Br..Br)	sum of geometrical distances between Br..Br	3D Atom Pairs
4822	G(Br..I)	sum of geometrical distances between Br..I	3D Atom Pairs
4823	G(I..I)	sum of geometrical distances between I..I	3D Atom Pairs
4824	qpmax	maximum positive charge	Charge descriptors
4825	qnmax	maximum negative charge	Charge descriptors
4826	Qpos	total positive charge	Charge descriptors
4827	Qneg	total negative charge	Charge descriptors
4828	Qtot	total absolute charge (electronic charge index - ECI)	Charge descriptors
4829	Qmean	mean absolute charge (charge polarization)	Charge descriptors
4830	Q2	total squared charge	Charge descriptors
4831	RPCG	relative positive charge	Charge descriptors
4832	RNCG	relative negative charge	Charge descriptors
4833	SPP	submolecular polarity parameter	Charge descriptors
4834	TE1	topographic electronic descriptor	Charge descriptors
4835	TE2	topographic electronic descriptor (bond restricted)	Charge descriptors
4836	PCWTE1	partial charge weighted topological electronic index	Charge descriptors
4837	PCWTE2	partial charge weighted topological electronic index (bond restricted)	Charge descriptors
4838	LDI	local dipole index	Charge descriptors
4839	Uc	unsaturation count	Molecular properties
4840	Ui	unsaturation index	Molecular properties
4841	Hy	hydrophilic factor	Molecular properties
4842	AMR	Ghose-Crippen molar refractivity	Molecular properties
4843	TPSA(NO)	topological polar surface area using N,O polar contributions	Molecular properties
4844	TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions	Molecular properties
4845	MLOGP	Moriguchi octanol-water partition coeff. (logP)	Molecular properties
4846	MLOGP2	squared Moriguchi octanol-water partition coeff. (logP <sup>2</sup> )	Molecular properties
4847	ALOGP	Ghose-Crippen octanol-water partition coeff. (logP)	Molecular properties
4848	ALOGP2	squared Ghose-Crippen octanol-water partition coeff. (logP <sup>2</sup> )	Molecular properties
4849	SAtot	total surface area from P_VSA-like descriptors	Molecular properties
4850	SAacc	surface area of acceptor atoms from P_VSA-like descriptors	Molecular properties
4851	SAdon	surface area of donor atoms from P_VSA-like descriptors	Molecular properties
4852	Vx	McGowan volume	Molecular properties
4853	VvdwMG	van der Waals volume from McGowan volume	Molecular properties
4854	VvdwZAZ	van der Waals volume from Zhao-Abraham-Zissimos equation	Molecular properties
4855	PDI	packing density index	Molecular properties
4856	BLTF96	Verhaar Fish base-line toxicity from MLOGP (mmol/l)	Molecular properties
4857	BLTD48	Verhaar Daphnia base-line toxicity from MLOGP (mmol/l)	Molecular properties
4858	BLTA96	Verhaar Algae base-line toxicity from MLOGP (mmol/l)	Molecular properties
4859	cRo5	Complementary Lipinski Alert index	Drug-like indices
4860	DLS_01	modified drug-like score from Lipinski (4 rules)	Drug-like indices
4861	DLS_02	modified drug-like score from Oprea et al. (6 rules)	Drug-like indices
4862	DLS_03	modified drug-like score from Walters et al. (6 rules)	Drug-like indices
4863	DLS_04	modified drug-like score from Chen et al. (7 rules)	Drug-like indices
4864	DLS_05	modified drug-like score from Zheng et al. (2 rules)	Drug-like indices
4865	DLS_06	modified drug-like score from Rishton (6 rules)	Drug-like indices
4866	DLS_07	modified drug-like score from Veber et al. (2 rules)	Drug-like indices
4867	DLS_cons	DRAGON consensus drug-like score	Drug-like indices
4868	LLS_01	modified lead-like score from Congreve et al. (6 rules)	Drug-like indices
4869	LLS_02	modified lead-like score from Monge et al. (8 rules)	Drug-like indices
4870	CMC-80	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 80%	Drug-like indices
4871	CMC-50	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 50%	Drug-like indices
4872	Inflammat-80	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80%	Drug-like indices
4873	Inflammat-50	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50%	Drug-like indices
4874	Depressant-80	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80%	Drug-like indices
4875	Depressant-50	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50%	Drug-like indices
4876	Psychotic-80	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80%	Drug-like indices
4877	Psychotic-50	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50%	Drug-like indices
4878	Hypertens-80	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80%	Drug-like indices
4879	Hypertens-50	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50%	Drug-like indices
4880	Hypnotic-80	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80%	Drug-like indices
4881	Hypnotic-50	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50%	Drug-like indices
4882	Neoplastic-80	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80%	Drug-like indices
4883	Neoplastic-50	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50%	Drug-like indices
4884	Infective-80	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80%	Drug-like indices
4885	Infective-50	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50%	Drug-like indices