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Complete list of descriptors calculated by Dragon 7

Following, the complete list of all descriptors available in **Dragon 7**, grouped by block:

No.	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	**GD**	graph density	Constitutional indices
12	**nAT**	number of atoms	Constitutional indices
13	**nSK**	number of non-H atoms	Constitutional indices
14	**nTA**	number of terminal atoms	Constitutional indices
15	**nBT**	number of bonds	Constitutional indices
16	**nBO**	number of non-H bonds	Constitutional indices
17	**nBM**	number of multiple bonds	Constitutional indices
18	**SCBO**	sum of conventional bond orders (H-depleted)	Constitutional indices
19	**RBN**	number of rotatable bonds	Constitutional indices

No.	Name	Description	Block
20	**RBF**	rotatable bond fraction	Constitutional indices
21	**nDB**	number of double bonds	Constitutional indices
22	**nTB**	number of triple bonds	Constitutional indices
23	**nAB**	number of aromatic bonds	Constitutional indices
24	**nH**	number of Hydrogen atoms	Constitutional indices
25	**nC**	number of Carbon atoms	Constitutional indices
26	**nN**	number of Nitrogen atoms	Constitutional indices
27	**nO**	number of Oxygen atoms	Constitutional indices
28	**nP**	number of Phosphorous atoms	Constitutional indices
29	**nS**	number of Sulfur atoms	Constitutional indices
30	**nF**	number of Fluorine atoms	Constitutional indices
31	**nCL**	number of Chlorine atoms	Constitutional indices
32	**nBR**	number of Bromine atoms	Constitutional indices
33	**nI**	number of Iodine atoms	Constitutional indices
34	**nB**	number of Boron atoms	Constitutional indices
35	**nHM**	number of heavy atoms	Constitutional indices
36	**nHet**	number of heteroatoms	Constitutional indices
37	**nX**	number of halogen atoms	Constitutional indices
38	**H%**	percentage of H atoms	Constitutional indices

No.	Name	Description	Block
39	**C%**	percentage of C atoms	Constitutional indices
40	**N%**	percentage of N atoms	Constitutional indices
41	**O%**	percentage of O atoms	Constitutional indices
42	**X%**	percentage of halogen atoms	Constitutional indices
43	**nCsp3**	number of sp3 hybridized Carbon atoms	Constitutional indices
44	**nCsp2**	number of sp2 hybridized Carbon atoms	Constitutional indices
45	**nCsp**	number of sp hybridized Carbon atoms	Constitutional indices
46	**nStructures**	number of disconnected structures	Constitutional indices
47	**totalcharge**	total charge	Constitutional indices
48	**nCIC**	number of rings (cyclomatic number)	Ring descriptors
49	**nCIR**	number of circuits	Ring descriptors
50	**TRS**	total ring size	Ring descriptors
51	**Rperim**	ring perimeter	Ring descriptors
52	**Rbrid**	ring bridge count	Ring descriptors
53	**MCD**	molecular cyclized degree	Ring descriptors
54	**RFD**	ring fusion density	Ring descriptors
55	**RCI**	ring complexity index	Ring descriptors
56	**NRS**	number of ring systems	Ring descriptors
57	**NNRS**	normalized number of ring systems	Ring descriptors

No.	Name	Description	Block
58	**nR03**	number of 3-membered rings	Ring descriptors
59	**nR04**	number of 4-membered rings	Ring descriptors
60	**nR05**	number of 5-membered rings	Ring descriptors
61	**nR06**	number of 6-membered rings	Ring descriptors
62	**nR07**	number of 7-membered rings	Ring descriptors
63	**nR08**	number of 8-membered rings	Ring descriptors
64	**nR09**	number of 9-membered rings	Ring descriptors
65	**nR10**	number of 10-membered rings	Ring descriptors
66	**nR11**	number of 11-membered rings	Ring descriptors
67	**nR12**	number of 12-membered rings	Ring descriptors
68	**nBnz**	number of benzene-like rings	Ring descriptors
69	**ARR**	aromatic ratio	Ring descriptors
70	**D/Dtr03**	distance/detour ring index of order 3	Ring descriptors
71	**D/Dtr04**	distance/detour ring index of order 4	Ring descriptors
72	**D/Dtr05**	distance/detour ring index of order 5	Ring descriptors
73	**D/Dtr06**	distance/detour ring index of order 6	Ring descriptors
74	**D/Dtr07**	distance/detour ring index of order 7	Ring descriptors
75	**D/Dtr08**	distance/detour ring index of order 8	Ring descriptors
76	**D/Dtr09**	distance/detour ring index of order 9	Ring descriptors

No.	Name	Description	Block
77	**D/Dtr10**	distance/detour ring index of order 10	Ring descriptors
78	**D/Dtr11**	distance/detour ring index of order 11	Ring descriptors
79	**D/Dtr12**	distance/detour ring index of order 12	Ring descriptors
80	**ZM1**	first Zagreb index	Topological indices
81	**ZM1V**	first Zagreb index by valence vertex degrees	Topological indices
82	**ZM1Kup**	first Zagreb index by Kupchik vertex degrees	Topological indices
83	**ZM1Mad**	first Zagreb index by Madan vertex degrees	Topological indices
84	**ZM1Per**	first Zagreb index by perturbation vertex degrees	Topological indices
85	**ZM1MulPer**	first Zagreb index by multiplicative perturbation vertex degrees	Topological indices
86	**ZM2**	second Zagreb index	Topological indices
87	**ZM2V**	second Zagreb index by valence vertex degrees	Topological indices
88	**ZM2Kup**	second Zagreb index by Kupchik vertex degrees	Topological indices
89	**ZM2Mad**	second Zagreb index by Madan vertex degrees	Topological indices
90	**ZM2Per**	second Zagreb index by perturbation vertex degrees	Topological indices
91	**ZM2MulPer**	second Zagreb index by multiplicative perturbation vertex degrees	Topological indices
92	**ON0**	overall modified Zagreb index of order 0	Topological indices
93	**ON0V**	overall modified Zagreb index of order 0 by valence vertex degrees	Topological indices
94	**ON1**	overall modified Zagreb index of order 1	Topological indices
95	**ON1V**	overall modified Zagreb index of order 1 by valence vertex degrees	Topological indices

No.	Name	Description	Block
96	**Qindex**	quadratic index	Topological indices
97	**BBI**	Bertz branching index	Topological indices
98	**DBI**	Dragon branching index	Topological indices
99	**SNar**	Narumi simple topological index (log function)	Topological indices
100	**HNar**	Narumi harmonic topological index	Topological indices
101	**GNar**	Narumi geometric topological index	Topological indices
102	**Xt**	total structure connectivity index	Topological indices
103	**Dz**	Pogliani index	Topological indices
104	**Ram**	ramification index	Topological indices
105	**BLI**	Kier benzene-likeliness index	Topological indices
106	**Pol**	polarity number	Topological indices
107	**LPRS**	log of product of row sums (PRS)	Topological indices
108	**MSD**	mean square distance index (Balaban)	Topological indices
109	**SPI**	superpendentic index	Topological indices
110	**PJI2**	2D Petitjean shape index	Topological indices
111	**ECC**	eccentricity	Topological indices
112	**AECC**	average eccentricity	Topological indices
113	**DECC**	eccentric	Topological indices
114	**MDDD**	mean distance degree deviation	Topological indices

No.	Name	Description	Block
115	**UNIP**	unipolarity	Topological indices
116	**CENT**	centralization	Topological indices
117	**VAR**	variation	Topological indices
118	**ICR**	radial centric information index	Topological indices
119	**SMTI**	Schultz Molecular Topological Index (MTI)	Topological indices
120	**SMTIV**	Schultz Molecular Topological Index by valence vertex degrees	Topological indices
121	**GMTI**	Gutman Molecular Topological Index	Topological indices
122	**GMTIV**	Gutman Molecular Topological Index by valence vertex degrees	Topological indices
123	**Xu**	Xu index	Topological indices
124	**CSI**	eccentric connectivity index	Topological indices
125	**Wap**	all-path Wiener index	Topological indices
126	**S1K**	1-path Kier alpha-modified shape index	Topological indices
127	**S2K**	2-path Kier alpha-modified shape index	Topological indices
128	**S3K**	3-path Kier alpha-modified shape index	Topological indices
129	**PHI**	Kier flexibility index	Topological indices
130	**PW2**	path/walk 2 - Randic shape index	Topological indices
131	**PW3**	path/walk 3 - Randic shape index	Topological indices
132	**PW4**	path/walk 4 - Randic shape index	Topological indices
133	**PW5**	path/walk 5 - Randic shape index	Topological indices

No.	Name	Description	Block
134	**MAXDN**	maximal electrotopological negative variation	Topological indices
135	**MAXDP**	maximal electrotopological positive variation	Topological indices
136	**DELS**	molecular electrotopological variation	Topological indices
137	**TIE**	E-state topological parameter	Topological indices
138	**Psi_i_s**	intrinsic state pseudoconnectivity index - type S	Topological indices
139	**Psi_i_A**	intrinsic state pseudoconnectivity index - type S average	Topological indices
140	**Psi_i_0**	intrinsic state pseudoconnectivity index - type 0	Topological indices
141	**Psi_i_1**	intrinsic state pseudoconnectivity index - type 1	Topological indices
142	**Psi_i_t**	intrinsic state pseudoconnectivity index - type T	Topological indices
143	**Psi_i_0d**	intrinsic state pseudoconnectivity index - type 0d	Topological indices
144	**Psi_i_1d**	intrinsic state pseudoconnectivity index - type 1d	Topological indices
145	**Psi_i_1s**	intrinsic state pseudoconnectivity index - type 1s	Topological indices
146	**Psi_e_A**	electrotopological state pseudoconnectivity index - type S average	Topological indices
147	**Psi_e_0**	electrotopological state pseudoconnectivity index - type 0	Topological indices
148	**Psi_e_1**	electrotopological state pseudoconnectivity index - type 1	Topological indices
149	**Psi_e_t**	electrotopological state pseudoconnectivity index - type T	Topological indices
150	**Psi_e_0d**	electrotopological state pseudoconnectivity index - type 0d	Topological indices
151	**Psi_e_1d**	electrotopological state pseudoconnectivity index - type 1d	Topological indices
152	**Psi_e_1s**	electrotopological state pseudoconnectivity index - type 1s	Topological indices

No.	Name	Description	Block
153	**BAC**	Balaban centric index	Topological indices
154	**LOC**	lopping centric index	Topological indices
155	**MWC01**	molecular walk count of order 1	Walk and path counts
156	**MWC02**	molecular walk count of order 2	Walk and path counts
157	**MWC03**	molecular walk count of order 3	Walk and path counts
158	**MWC04**	molecular walk count of order 4	Walk and path counts
159	**MWC05**	molecular walk count of order 5	Walk and path counts
160	**MWC06**	molecular walk count of order 6	Walk and path counts
161	**MWC07**	molecular walk count of order 7	Walk and path counts
162	**MWC08**	molecular walk count of order 8	Walk and path counts
163	**MWC09**	molecular walk count of order 9	Walk and path counts
164	**MWC10**	molecular walk count of order 10	Walk and path counts
165	**SRW02**	self-returning walk count of order 2	Walk and path counts
166	**SRW03**	self-returning walk count of order 3	Walk and path counts
167	**SRW04**	self-returning walk count of order 4	Walk and path counts
168	**SRW05**	self-returning walk count of order 5	Walk and path counts
169	**SRW06**	self-returning walk count of order 6	Walk and path counts
170	**SRW07**	self-returning walk count of order 7	Walk and path counts
171	**SRW08**	self-returning walk count of order 8	Walk and path counts

No.	Name	Description	Block
172	**SRW09**	self-returning walk count of order 9	Walk and path counts
173	**SRW10**	self-returning walk count of order 10	Walk and path counts
174	**MPC01**	molecular path count of order 1 (no. of non-H bonds)	Walk and path counts
175	**MPC02**	molecular path count of order 2 (Gordon-Scantlebury index)	Walk and path counts
176	**MPC03**	molecular path count of order 3	Walk and path counts
177	**MPC04**	molecular path count of order 4	Walk and path counts
178	**MPC05**	molecular path count of order 5	Walk and path counts
179	**MPC06**	molecular path count of order 6	Walk and path counts
180	**MPC07**	molecular path count of order 7	Walk and path counts
181	**MPC08**	molecular path count of order 8	Walk and path counts
182	**MPC09**	molecular path count of order 9	Walk and path counts
183	**MPC10**	molecular path count of order 10	Walk and path counts
184	**piPC01**	molecular multiple path count of order 1	Walk and path counts
185	**piPC02**	molecular multiple path count of order 2	Walk and path counts
186	**piPC03**	molecular multiple path count of order 3	Walk and path counts
187	**piPC04**	molecular multiple path count of order 4	Walk and path counts
188	**piPC05**	molecular multiple path count of order 5	Walk and path counts
189	**piPC06**	molecular multiple path count of order 6	Walk and path counts
190	**piPC07**	molecular multiple path count of order 7	Walk and path counts

No.	Name	Description	Block
191	**piPC08**	molecular multiple path count of order 8	Walk and path counts
192	**piPC09**	molecular multiple path count of order 9	Walk and path counts
193	**piPC10**	molecular multiple path count of order 10	Walk and path counts
194	**TWC**	total walk count	Walk and path counts
195	**TPC**	total path count	Walk and path counts
196	**piID**	conventional bond order ID number	Walk and path counts
197	**PCR**	ratio of multiple path count over path count	Walk and path counts
198	**PCD**	difference between multiple path count and path count	Walk and path counts
199	**CID**	Randic ID number	Walk and path counts
200	**BID**	Balaban ID number	Walk and path counts
201	**X0**	connectivity index of order 0	Connectivity indices
202	**X1**	connectivity index of order 1 (Randic connectivity index)	Connectivity indices
203	**X2**	connectivity index of order 2	Connectivity indices
204	**X3**	connectivity index of order 3	Connectivity indices
205	**X4**	connectivity index of order 4	Connectivity indices
206	**X5**	connectivity index of order 5	Connectivity indices
207	**X0A**	average connectivity index of order 0	Connectivity indices
208	**X1A**	average connectivity index of order 1	Connectivity indices
209	**X2A**	average connectivity index of order 2	Connectivity indices

No.	Name	Description	Block
210	**X3A**	average connectivity index of order 3	Connectivity indices
211	**X4A**	average connectivity index of order 4	Connectivity indices
212	**X5A**	average connectivity index of order 5	Connectivity indices
213	**X0v**	valence connectivity index of order 0	Connectivity indices
214	**X1v**	valence connectivity index of order 1	Connectivity indices
215	**X2v**	valence connectivity index of order 2	Connectivity indices
216	**X3v**	valence connectivity index of order 3	Connectivity indices
217	**X4v**	valence connectivity index of order 4	Connectivity indices
218	**X5v**	valence connectivity index of order 5	Connectivity indices
219	**X0Av**	average valence connectivity index of order 0	Connectivity indices
220	**X1Av**	average valence connectivity index of order 1	Connectivity indices
221	**X2Av**	average valence connectivity index of order 2	Connectivity indices
222	**X3Av**	average valence connectivity index of order 3	Connectivity indices
223	**X4Av**	average valence connectivity index of order 4	Connectivity indices
224	**X5Av**	average valence connectivity index of order 5	Connectivity indices
225	**X0sol**	solvation connectivity index of order 0	Connectivity indices
226	**X1sol**	solvation connectivity index of order 1	Connectivity indices
227	**X2sol**	solvation connectivity index of order 2	Connectivity indices
228	**X3sol**	solvation connectivity index of order 3	Connectivity indices

No.	Name	Description	Block
229	**X4sol**	solvation connectivity index of order 4	Connectivity indices
230	**X5sol**	solvation connectivity index of order 5	Connectivity indices
231	**XMOD**	modified Randic index	Connectivity indices
232	**RDCHI**	reciprocal distance sum Randic-like index	Connectivity indices
233	**RDSQ**	reciprocal distance sum inverse Randic-like index	Connectivity indices
234	**X1Kup**	Kupchik connectivity index	Connectivity indices
235	**X1Mad**	connectivity topochemical index	Connectivity indices
236	**X1Per**	perturbation connectivity index	Connectivity indices
237	**X1MulPer**	multiplicative perturbation connectivity index	Connectivity indices
238	**ISIZ**	information index on molecular size	Information indices
239	**IAC**	total information index on atomic composition	Information indices
240	**AAC**	mean information index on atomic composition	Information indices
241	**IDE**	mean information content on the distance equality	Information indices
242	**IDM**	mean information content on the distance magnitude	Information indices
243	**IDDE**	mean information content on the distance degree equality	Information indices
244	**IDDM**	mean information content on the distance degree magnitude	Information indices
245	**IDET**	total information content on the distance equality	Information indices
246	**IDMT**	total information content on the distance magnitude	Information indices
247	**IVDE**	mean information content on the vertex degree equality	Information indices

No.	Name	Description	Block
248	**IVDM**	mean information content on the vertex degree magnitude	Information indices
249	**Ges**	Number of symmetry classes (based on electrotopological state)	Information indices
250	**rGes**	Relative number of symmetry classes (based on electrotopological state)	Information indices
251	**S0K**	Kier symmetry index	Information indices
252	**HVcpx**	graph vertex complexity index	Information indices
253	**HDcpx**	graph distance complexity index (log function)	Information indices
254	**Uindex**	Balaban U index	Information indices
255	**Vindex**	Balaban V index	Information indices
256	**Xindex**	Balaban X index	Information indices
257	**Yindex**	Balaban Y index	Information indices
258	**IC0**	Information Content index (neighborhood symmetry of 0-order)	Information indices
259	**IC1**	Information Content index (neighborhood symmetry of 1-order)	Information indices
260	**IC2**	Information Content index (neighborhood symmetry of 2-order)	Information indices
261	**IC3**	Information Content index (neighborhood symmetry of 3-order)	Information indices
262	**IC4**	Information Content index (neighborhood symmetry of 4-order)	Information indices
263	**IC5**	Information Content index (neighborhood symmetry of 5-order)	Information indices
264	**TIC0**	Total Information Content index (neighborhood symmetry of 0-order)	Information indices
265	**TIC1**	Total Information Content index (neighborhood symmetry of 1-order)	Information indices
266	**TIC2**	Total Information Content index (neighborhood symmetry of 2-order)	Information indices

No.	Name	Description	Block
267	**TIC3**	Total Information Content index (neighborhood symmetry of 3-order)	Information indices
268	**TIC4**	Total Information Content index (neighborhood symmetry of 4-order)	Information indices
269	**TIC5**	Total Information Content index (neighborhood symmetry of 5-order)	Information indices
270	**SIC0**	Structural Information Content index (neighborhood symmetry of 0-order)	Information indices
271	**SIC1**	Structural Information Content index (neighborhood symmetry of 1-order)	Information indices
272	**SIC2**	Structural Information Content index (neighborhood symmetry of 2-order)	Information indices
273	**SIC3**	Structural Information Content index (neighborhood symmetry of 3-order)	Information indices
274	**SIC4**	Structural Information Content index (neighborhood symmetry of 4-order)	Information indices
275	**SIC5**	Structural Information Content index (neighborhood symmetry of 5-order)	Information indices
276	**CIC0**	Complementary Information Content index (neighborhood symmetry of 0-order)	Information indices
277	**CIC1**	Complementary Information Content index (neighborhood symmetry of 1-order)	Information indices
278	**CIC2**	Complementary Information Content index (neighborhood symmetry of 2-order)	Information indices
279	**CIC3**	Complementary Information Content index (neighborhood symmetry of 3-order)	Information indices
280	**CIC4**	Complementary Information Content index (neighborhood symmetry of 4-order)	Information indices
281	**CIC5**	Complementary Information Content index (neighborhood symmetry of 5-order)	Information indices
282	**BIC0**	Bond Information Content index (neighborhood symmetry of 0-order)	Information indices
283	**BIC1**	Bond Information Content index (neighborhood symmetry of 1-order)	Information indices
284	**BIC2**	Bond Information Content index (neighborhood symmetry of 2-order)	Information indices
285	**BIC3**	Bond Information Content index (neighborhood symmetry of 3-order)	Information indices

No.	Name	Description	Block
286	**BIC4**	Bond Information Content index (neighborhood symmetry of 4-order)	Information indices
287	**BIC5**	Bond Information Content index (neighborhood symmetry of 5-order)	Information indices
288	**J_A**	Balaban-like index from adjacency matrix	2D matrix-based descriptors
289	**SpPos_A**	spectral positive sum from adjacency matrix	2D matrix-based descriptors
290	**SpPosA_A**	normalized spectral positive sum from adjacency matrix	2D matrix-based descriptors
291	**SpPosLog_A**	logarithmic spectral positive sum from adjacency matrix	2D matrix-based descriptors
292	**SpMax_A**	leading eigenvalue from adjacency matrix (Lovasz-Pelikan index)	2D matrix-based descriptors
293	**SpMaxA_A**	normalized leading eigenvalue from adjacency matrix	2D matrix-based descriptors
294	**SpDiam_A**	spectral diameter from adjacency matrix	2D matrix-based descriptors
295	**SpAD_A**	spectral absolute deviation from adjacency matrix	2D matrix-based descriptors
296	**SpMAD_A**	spectral mean absolute deviation from adjacency matrix	2D matrix-based descriptors
297	**Ho_A**	Hosoya-like index (log function) from adjacency matrix	2D matrix-based descriptors
298	**EE_A**	Estrada-like index (log function) from adjacency matrix	2D matrix-based descriptors
299	**VE1_A**	coefficient sum of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors

No.	Name	Description	Block
300	**VE2_A**	average coefficient of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors
301	**VE3_A**	logarithmic coefficient sum of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors
302	**VE1sign_A**	coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
303	**VE2sign_A**	average coefficient of the last eigenvector from adjacency matrix	2D matrix-based descriptors
304	**VE3sign_A**	logarithmic coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
305	**VR1_A**	Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
306	**VR2_A**	normalized Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
307	**VR3_A**	logarithmic Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
308	**Wi_D**	Wiener-like index from topological distance matrix (Wiener index)	2D matrix-based descriptors
309	**WiA_D**	average Wiener-like index from topological distance matrix	2D matrix-based descriptors
310	**AVS_D**	average vertex sum from topological distance matrix	2D matrix-based descriptors
311	**H_D**	Harary-like index from topological distance matrix (Harary index)	2D matrix-based descriptors
312	**Chi_D**	Randic-like index from topological distance matrix	2D matrix-based descriptors
313	**ChiA_D**	average Randic-like index from topological distance matrix	2D matrix-based descriptors

No.	Name	Description	Block
314	**J_D**	Balaban-like index from topological distance matrix (Balaban distance connectivity index)	2D matrix-based descriptors
315	**HyWi_D**	hyper-Wiener-like index (log function) from topological distance matrix	2D matrix-based descriptors
316	**SpPos_D**	spectral positive sum from topological distance matrix	2D matrix-based descriptors
317	**SpPosA_D**	normalized spectral positive sum from topological distance matrix	2D matrix-based descriptors
318	**SpPosLog_D**	logarithmic spectral positive sum from topological distance matrix	2D matrix-based descriptors
319	**SpMax_D**	leading eigenvalue from topological distance matrix	2D matrix-based descriptors
320	**SpMaxA_D**	normalized leading eigenvalue from topological distance matrix	2D matrix-based descriptors
321	**SpDiam_D**	spectral diameter from topological distance matrix	2D matrix-based descriptors
322	**SpAD_D**	spectral absolute deviation from topological distance matrix	2D matrix-based descriptors
323	**SpMAD_D**	spectral mean absolute deviation from topological distance matrix	2D matrix-based descriptors
324	**Ho_D**	Hosoya-like index (log function) from topological distance matrix	2D matrix-based descriptors
325	**EE_D**	Estrada-like index (log function) from topological distance matrix	2D matrix-based descriptors
326	**SM2_D**	spectral moment of order 2 from topological distance matrix	2D matrix-based descriptors
327	**SM3_D**	spectral moment of order 3 from topological distance matrix	2D matrix-based descriptors

No.	Name	Description	Block
328	**SM4_D**	spectral moment of order 4 from topological distance matrix	2D matrix-based descriptors
329	**SM5_D**	spectral moment of order 5 from topological distance matrix	2D matrix-based descriptors
330	**SM6_D**	spectral moment of order 6 from topological distance matrix	2D matrix-based descriptors
331	**VE1_D**	coefficient sum of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors
332	**VE2_D**	average coefficient of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors
333	**VE3_D**	logarithmic coefficient sum of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors
334	**VE1sign_D**	coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
335	**VE2sign_D**	average coefficient of the last eigenvector from topological distance matrix	2D matrix-based descriptors
336	**VE3sign_D**	logarithmic coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
337	**VR1_D**	Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
338	**VR2_D**	normalized Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
339	**VR3_D**	logarithmic Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
340	**QW_L**	quasi-Wiener index (Kirchhoff number) from Laplace matrix	2D matrix-based descriptors
341	**TI1_L**	first Mohar index from Laplace matrix	2D matrix-based descriptors

No.	Name	Description	Block
342	**TI2_L**	second Mohar index from Laplace matrix	2D matrix-based descriptors
343	**STN_L**	spanning tree number (log function) from Laplace matrix	2D matrix-based descriptors
344	**SpPos_L**	spectral positive sum from Laplace matrix	2D matrix-based descriptors
345	**SpPosA_L**	normalized spectral positive sum from Laplace matrix	2D matrix-based descriptors
346	**SpPosLog_L**	logarithmic spectral positive sum from Laplace matrix	2D matrix-based descriptors
347	**SpMax_L**	leading eigenvalue from Laplace matrix	2D matrix-based descriptors
348	**SpMaxA_L**	normalized leading eigenvalue from Laplace matrix	2D matrix-based descriptors
349	**SpDiam_L**	spectral diameter from Laplace matrix	2D matrix-based descriptors
350	**SpAD_L**	spectral absolute deviation from Laplace matrix	2D matrix-based descriptors
351	**SpMAD_L**	spectral mean absolute deviation from Laplace matrix	2D matrix-based descriptors
352	**Ho_L**	Hosoya-like index (log function) from Laplace matrix	2D matrix-based descriptors
353	**EE_L**	Estrada-like index (log function) from Laplace matrix	2D matrix-based descriptors
354	**SM2_L**	spectral moment of order 2 from Laplace matrix	2D matrix-based descriptors
355	**SM3_L**	spectral moment of order 3 from Laplace matrix	2D matrix-based descriptors

No.	Name	Description	Block
356	**SM4_L**	spectral moment of order 4 from Laplace matrix	2D matrix-based descriptors
357	**SM5_L**	spectral moment of order 5 from Laplace matrix	2D matrix-based descriptors
358	**SM6_L**	spectral moment of order 6 from Laplace matrix	2D matrix-based descriptors
359	**VE1_L**	coefficient sum of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors
360	**VE2_L**	average coefficient of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors
361	**VE3_L**	logarithmic coefficient sum of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors
362	**VE1sign_L**	coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
363	**VE2sign_L**	average coefficient of the last eigenvector from Laplace matrix	2D matrix-based descriptors
364	**VE3sign_L**	logarithmic coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
365	**VR1_L**	Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
366	**VR2_L**	normalized Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
367	**VR3_L**	logarithmic Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
368	**AVS_X**	average vertex sum from chi matrix	2D matrix-based descriptors
369	**H_X**	Harary-like index from chi matrix	2D matrix-based descriptors

No.	Name	Description	Block
370	**Chi_X**	Randic-like index from chi matrix	2D matrix-based descriptors
371	**ChiA_X**	average Randic-like index from chi matrix	2D matrix-based descriptors
372	**J_X**	Balaban-like index from chi matrix	2D matrix-based descriptors
373	**HyWi_X**	hyper-Wiener-like index (log function) from chi matrix	2D matrix-based descriptors
374	**SpPos_X**	spectral positive sum from chi matrix	2D matrix-based descriptors
375	**SpPosA_X**	normalized spectral positive sum from chi matrix	2D matrix-based descriptors
376	**SpPosLog_X**	logarithmic spectral positive sum from chi matrix	2D matrix-based descriptors
377	**SpMax_X**	leading eigenvalue from chi matrix	2D matrix-based descriptors
378	**SpMaxA_X**	normalized leading eigenvalue from chi matrix	2D matrix-based descriptors
379	**SpDiam_X**	spectral diameter from chi matrix	2D matrix-based descriptors
380	**SpAD_X**	spectral absolute deviation from chi matrix	2D matrix-based descriptors
381	**SpMAD_X**	spectral mean absolute deviation from chi matrix	2D matrix-based descriptors
382	**Ho_X**	Hosoya-like index (log function) from chi matrix	2D matrix-based descriptors
383	**EE_X**	Estrada-like index (log function) from chi matrix	2D matrix-based descriptors

No.	Name	Description	Block
384	**SM2_X**	spectral moment of order 2 from chi matrix	2D matrix-based descriptors
385	**SM3_X**	spectral moment of order 3 from chi matrix	2D matrix-based descriptors
386	**SM4_X**	spectral moment of order 4 from chi matrix	2D matrix-based descriptors
387	**SM5_X**	spectral moment of order 5 from chi matrix	2D matrix-based descriptors
388	**SM6_X**	spectral moment of order 6 from chi matrix	2D matrix-based descriptors
389	**VE1_X**	coefficient sum of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors
390	**VE2_X**	average coefficient of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors
391	**VE3_X**	logarithmic coefficient sum of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors
392	**VE1sign_X**	coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
393	**VE2sign_X**	average coefficient of the last eigenvector from chi matrix	2D matrix-based descriptors
394	**VE3sign_X**	logarithmic coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
395	**VR1_X**	Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
396	**VR2_X**	normalized Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
397	**VR3_X**	logarithmic Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors

No.	Name	Description	Block
398	**Wi_H2**	Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors
399	**WiA_H2**	average Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors
400	**AVS_H2**	average vertex sum from reciprocal squared distance matrix	2D matrix-based descriptors
401	**Chi_H2**	Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
402	**ChiA_H2**	average Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
403	**J_H2**	Balaban-like index from reciprocal squared distance matrix	2D matrix-based descriptors
404	**HyWi_H2**	hyper-Wiener-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
405	**SpPos_H2**	spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
406	**SpPosA_H2**	normalized spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
407	**SpPosLog_H2**	logarithmic spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
408	**SpMax_H2**	leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
409	**SpMaxA_H2**	normalized leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
410	**SpDiam_H2**	spectral diameter from reciprocal squared distance matrix	2D matrix-based descriptors
411	**SpAD_H2**	spectral absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors

No.	Name	Description	Block
412	**SpMAD_H2**	spectral mean absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors
413	**Ho_H2**	Hosoya-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
414	**EE_H2**	Estrada-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
415	**SM2_H2**	spectral moment of order 2 from reciprocal squared distance matrix	2D matrix-based descriptors
416	**SM3_H2**	spectral moment of order 3 from reciprocal squared distance matrix	2D matrix-based descriptors
417	**SM4_H2**	spectral moment of order 4 from reciprocal squared distance matrix	2D matrix-based descriptors
418	**SM5_H2**	spectral moment of order 5 from reciprocal squared distance matrix	2D matrix-based descriptors
419	**SM6_H2**	spectral moment of order 6 from reciprocal squared distance matrix	2D matrix-based descriptors
420	**VE1_H2**	coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors
421	**VE2_H2**	average coefficient of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors
422	**VE3_H2**	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors
423	**VE1sign_H2**	coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
424	**VE2sign_H2**	average coefficient of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
425	**VE3sign_H2**	logarithmic coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors

No.	Name	Description	Block
426	**VR1_H2**	Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
427	**VR2_H2**	normalized Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
428	**VR3_H2**	logarithmic Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
429	**Wi_Dt**	Wiener-like index from detour matrix (detour index)	2D matrix-based descriptors
430	**WiA_Dt**	average Wiener-like index from detour matrix	2D matrix-based descriptors
431	**AVS_Dt**	average vertex sum from detour matrix	2D matrix-based descriptors
432	**H_Dt**	Harary-like index from detour matrix	2D matrix-based descriptors
433	**Chi_Dt**	Randic-like index from detour matrix	2D matrix-based descriptors
434	**ChiA_Dt**	average Randic-like index from detour matrix	2D matrix-based descriptors
435	**J_Dt**	Balaban-like index from detour matrix	2D matrix-based descriptors
436	**HyWi_Dt**	hyper-Wiener-like index (log function) from detour matrix	2D matrix-based descriptors
437	**SpPos_Dt**	spectral positive sum from detour matrix	2D matrix-based descriptors
438	**SpPosA_Dt**	normalized spectral positive sum from detour matrix	2D matrix-based descriptors
439	**SpPosLog_Dt**	logarithmic spectral positive sum from detour matrix	2D matrix-based descriptors

No.	Name	Description	Block
440	**SpMax_Dt**	leading eigenvalue from detour matrix	2D matrix-based descriptors
441	**SpMaxA_Dt**	normalized leading eigenvalue from detour matrix	2D matrix-based descriptors
442	**SpDiam_Dt**	spectral diameter from detour matrix	2D matrix-based descriptors
443	**SpAD_Dt**	spectral absolute deviation from detour matrix	2D matrix-based descriptors
444	**SpMAD_Dt**	spectral mean absolute deviation from detour matrix	2D matrix-based descriptors
445	**Ho_Dt**	Hosoya-like index (log function) from detour matrix	2D matrix-based descriptors
446	**EE_Dt**	Estrada-like index (log function) from detour matrix	2D matrix-based descriptors
447	**SM2_Dt**	spectral moment of order 2 from detour matrix	2D matrix-based descriptors
448	**SM3_Dt**	spectral moment of order 3 from detour matrix	2D matrix-based descriptors
449	**SM4_Dt**	spectral moment of order 4 from detour matrix	2D matrix-based descriptors
450	**SM5_Dt**	spectral moment of order 5 from detour matrix	2D matrix-based descriptors
451	**SM6_Dt**	spectral moment of order 6 from detour matrix	2D matrix-based descriptors
452	**VE1_Dt**	coefficient sum of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors
453	**VE2_Dt**	average coefficient of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors

No.	Name	Description	Block
454	**VE3_Dt**	logarithmic coefficient sum of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors
455	**VE1sign_Dt**	coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
456	**VE2sign_Dt**	average coefficient of the last eigenvector from detour matrix	2D matrix-based descriptors
457	**VE3sign_Dt**	logarithmic coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
458	**VR1_Dt**	Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
459	**VR2_Dt**	normalized Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
460	**VR3_Dt**	logarithmic Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
461	**Wi_D/Dt**	Wiener-like index from distance/detour matrix	2D matrix-based descriptors
462	**WiA_D/Dt**	average Wiener-like index from distance/detour matrix	2D matrix-based descriptors
463	**AVS_D/Dt**	average vertex sum from distance/detour matrix	2D matrix-based descriptors
464	**H_D/Dt**	Harary-like index from distance/detour matrix	2D matrix-based descriptors
465	**Chi_D/Dt**	Randic-like index from distance/detour matrix	2D matrix-based descriptors
466	**ChiA_D/Dt**	average Randic-like index from distance/detour matrix	2D matrix-based descriptors
467	**J_D/Dt**	Balaban-like index from distance/detour matrix	2D matrix-based descriptors

No.	Name	Description	Block
468	**HyWi_D/Dt**	hyper-Wiener-like index (log function) from distance/detour matrix	2D matrix-based descriptors
469	**SpPos_D/Dt**	spectral positive sum from distance/detour matrix	2D matrix-based descriptors
470	**SpPosA_D/Dt**	normalized spectral positive sum from distance/detour matrix	2D matrix-based descriptors
471	**SpPosLog_D/Dt**	logarithmic spectral positive sum from distance/detour matrix	2D matrix-based descriptors
472	**SpMax_D/Dt**	leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
473	**SpMaxA_D/Dt**	normalized leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
474	**SpDiam_D/Dt**	spectral diameter from distance/detour matrix	2D matrix-based descriptors
475	**SpAD_D/Dt**	spectral absolute deviation from distance/detour matrix	2D matrix-based descriptors
476	**SpMAD_D/Dt**	spectral mean absolute deviation from distance/detour matrix	2D matrix-based descriptors
477	**Ho_D/Dt**	Hosoya-like index (log function) from distance/detour matrix	2D matrix-based descriptors
478	**EE_D/Dt**	Estrada-like index (log function) from distance/detour matrix	2D matrix-based descriptors
479	**SM2_D/Dt**	spectral moment of order 2 from distance/detour matrix	2D matrix-based descriptors
480	**SM3_D/Dt**	spectral moment of order 3 from distance/detour matrix	2D matrix-based descriptors
481	**SM4_D/Dt**	spectral moment of order 4 from distance/detour matrix	2D matrix-based descriptors

No.	Name	Description	Block
482	**SM5_D/Dt**	spectral moment of order 5 from distance/detour matrix	2D matrix-based descriptors
483	**SM6_D/Dt**	spectral moment of order 6 from distance/detour matrix	2D matrix-based descriptors
484	**VE1_D/Dt**	coefficient sum of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors
485	**VE2_D/Dt**	average coefficient of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors
486	**VE3_D/Dt**	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors
487	**VE1sign_D/Dt**	coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
488	**VE2sign_D/Dt**	average coefficient of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
489	**VE3sign_D/Dt**	logarithmic coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
490	**VR1_D/Dt**	Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
491	**VR2_D/Dt**	normalized Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
492	**VR3_D/Dt**	logarithmic Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
493	**Wi_Dz(Z)**	Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
494	**WiA_Dz(Z)**	average Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
495	**AVS_Dz(Z)**	average vertex sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors

No.	Name	Description	Block
496	**H_Dz(Z)**	Harary-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
497	**Chi_Dz(Z)**	Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
498	**ChiA_Dz(Z)**	average Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
499	**J_Dz(Z)**	Balaban-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
500	**HyWi_Dz(Z)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
501	**SpAbs_Dz(Z)**	graph energy from Barysz matrix weighted by atomic number	2D matrix-based descriptors
502	**SpPos_Dz(Z)**	spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
503	**SpPosA_Dz(Z)**	normalized spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
504	**SpPosLog_Dz(Z)**	logarithmic spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
505	**SpMax_Dz(Z)**	leading eigenvalue from Barysz matrix weighted by atomic number	2D matrix-based descriptors
506	**SpMaxA_Dz(Z)**	normalized leading eigenvalue from Barysz matrix weighted by atomic number	2D matrix-based descriptors
507	**SpDiam_Dz(Z)**	spectral diameter from Barysz matrix weighted by atomic number	2D matrix-based descriptors
508	**SpAD_Dz(Z)**	spectral absolute deviation from Barysz matrix weighted by atomic number	2D matrix-based descriptors
509	**SpMAD_Dz(Z)**	spectral mean absolute deviation from Barysz matrix weighted by atomic number	2D matrix-based descriptors

No.	Name	Description	Block
510	**Ho_Dz(Z)**	Hosoya-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
511	**EE_Dz(Z)**	Estrada-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
512	**SM1_Dz(Z)**	spectral moment of order 1 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
513	**SM2_Dz(Z)**	spectral moment of order 2 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
514	**SM3_Dz(Z)**	spectral moment of order 3 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
515	**SM4_Dz(Z)**	spectral moment of order 4 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
516	**SM5_Dz(Z)**	spectral moment of order 5 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
517	**SM6_Dz(Z)**	spectral moment of order 6 from Barysz matrix weighted by atomic number	2D matrix-based descriptors
518	**VE1_Dz(Z)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
519	**VE2_Dz(Z)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
520	**VE3_Dz(Z)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
521	**VE1sign_Dz(Z)**	coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors
522	**VE2sign_Dz(Z)**	average coefficient of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors
523	**VE3sign_Dz(Z)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors

No.	Name	Description	Block
524	**VR1_Dz(Z)**	Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
525	**VR2_Dz(Z)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
526	**VR3_Dz(Z)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
527	**Wi_Dz(m)**	Wiener-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
528	**WiA_Dz(m)**	average Wiener-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
529	**AVS_Dz(m)**	average vertex sum from Barysz matrix weighted by mass	2D matrix-based descriptors
530	**H_Dz(m)**	Harary-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
531	**Chi_Dz(m)**	Randic-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
532	**ChiA_Dz(m)**	average Randic-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
533	**J_Dz(m)**	Balaban-like index from Barysz matrix weighted by mass	2D matrix-based descriptors
534	**HyWi_Dz(m)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors
535	**SpAbs_Dz(m)**	graph energy from Barysz matrix weighted by mass	2D matrix-based descriptors
536	**SpPos_Dz(m)**	spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors
537	**SpPosA_Dz(m)**	normalized spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors

No.	Name	Description	Block
538	**SpPosLog_Dz(m)**	logarithmic spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors
539	**SpMax_Dz(m)**	leading eigenvalue from Barysz matrix weighted by mass	2D matrix-based descriptors
540	**SpMaxA_Dz(m)**	normalized leading eigenvalue from Barysz matrix weighted by mass	2D matrix-based descriptors
541	**SpDiam_Dz(m)**	spectral diameter from Barysz matrix weighted by mass	2D matrix-based descriptors
542	**SpAD_Dz(m)**	spectral absolute deviation from Barysz matrix weighted by mass	2D matrix-based descriptors
543	**SpMAD_Dz(m)**	spectral mean absolute deviation from Barysz matrix weighted by mass	2D matrix-based descriptors
544	**Ho_Dz(m)**	Hosoya-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors
545	**EE_Dz(m)**	Estrada-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors
546	**SM1_Dz(m)**	spectral moment of order 1 from Barysz matrix weighted by mass	2D matrix-based descriptors
547	**SM2_Dz(m)**	spectral moment of order 2 from Barysz matrix weighted by mass	2D matrix-based descriptors
548	**SM3_Dz(m)**	spectral moment of order 3 from Barysz matrix weighted by mass	2D matrix-based descriptors
549	**SM4_Dz(m)**	spectral moment of order 4 from Barysz matrix weighted by mass	2D matrix-based descriptors
550	**SM5_Dz(m)**	spectral moment of order 5 from Barysz matrix weighted by mass	2D matrix-based descriptors
551	**SM6_Dz(m)**	spectral moment of order 6 from Barysz matrix weighted by mass	2D matrix-based descriptors

No.	Name	Description	Block
552	**VE1_Dz(m)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors
553	**VE2_Dz(m)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors
554	**VE3_Dz(m)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors
555	**VE1sign_Dz(m)**	coefficient sum of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors
556	**VE2sign_Dz(m)**	average coefficient of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors
557	**VE3sign_Dz(m)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors
558	**VR1_Dz(m)**	Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors
559	**VR2_Dz(m)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors
560	**VR3_Dz(m)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors
561	**Wi_Dz(v)**	Wiener-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
562	**WiA_Dz(v)**	average Wiener-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
563	**AVS_Dz(v)**	average vertex sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
564	**H_Dz(v)**	Harary-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
565	**Chi_Dz(v)**	Randic-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
566	**ChiA_Dz(v)**	average Randic-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
567	**J_Dz(v)**	Balaban-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
568	**HyWi_Dz(v)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
569	**SpAbs_Dz(v)**	graph energy from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
570	**SpPos_Dz(v)**	spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
571	**SpPosA_Dz(v)**	normalized spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
572	**SpPosLog_Dz(v)**	logarithmic spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
573	**SpMax_Dz(v)**	leading eigenvalue from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
574	**SpMaxA_Dz(v)**	normalized leading eigenvalue from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
575	**SpDiam_Dz(v)**	spectral diameter from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
576	**SpAD_Dz(v)**	spectral absolute deviation from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
577	**SpMAD_Dz(v)**	spectral mean absolute deviation from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
578	**Ho_Dz(v)**	Hosoya-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
579	**EE_Dz(v)**	Estrada-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
580	**SM1_Dz(v)**	spectral moment of order 1 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
581	**SM2_Dz(v)**	spectral moment of order 2 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
582	**SM3_Dz(v)**	spectral moment of order 3 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
583	**SM4_Dz(v)**	spectral moment of order 4 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
584	**SM5_Dz(v)**	spectral moment of order 5 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
585	**SM6_Dz(v)**	spectral moment of order 6 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
586	**VE1_Dz(v)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
587	**VE2_Dz(v)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
588	**VE3_Dz(v)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
589	**VE1sign_Dz(v)**	coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
590	**VE2sign_Dz(v)**	average coefficient of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
591	**VE3sign_Dz(v)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
592	**VR1_Dz(v)**	Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
593	**VR2_Dz(v)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
594	**VR3_Dz(v)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors
595	**Wi_Dz(e)**	Wiener-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
596	**WiA_Dz(e)**	average Wiener-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
597	**AVS_Dz(e)**	average vertex sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
598	**H_Dz(e)**	Harary-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
599	**Chi_Dz(e)**	Randic-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
600	**ChiA_Dz(e)**	average Randic-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
601	**J_Dz(e)**	Balaban-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
602	**HyWi_Dz(e)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
603	**SpAbs_Dz(e)**	graph energy from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
604	**SpPos_Dz(e)**	spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
605	**SpPosA_Dz(e)**	normalized spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
606	**SpPosLog_Dz(e)**	logarithmic spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
607	**SpMax_Dz(e)**	leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors

No.	Name	Description	Block
608	**SpMaxA_Dz(e)**	normalized leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
609	**SpDiam_Dz(e)**	spectral diameter from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
610	**SpAD_Dz(e)**	spectral absolute deviation from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
611	**SpMAD_Dz(e)**	spectral mean absolute deviation from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
612	**Ho_Dz(e)**	Hosoya-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
613	**EE_Dz(e)**	Estrada-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
614	**SM1_Dz(e)**	spectral moment of order 1 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
615	**SM2_Dz(e)**	spectral moment of order 2 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
616	**SM3_Dz(e)**	spectral moment of order 3 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
617	**SM4_Dz(e)**	spectral moment of order 4 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
618	**SM5_Dz(e)**	spectral moment of order 5 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
619	**SM6_Dz(e)**	spectral moment of order 6 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
620	**VE1_Dz(e)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
621	**VE2_Dz(e)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors

No.	Name	Description	Block
622	**VE3_Dz(e)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
623	**VE1sign_Dz(e)**	coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
624	**VE2sign_Dz(e)**	average coefficient of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
625	**VE3sign_Dz(e)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
626	**VR1_Dz(e)**	Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
627	**VR2_Dz(e)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
628	**VR3_Dz(e)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
629	**Wi_Dz(p)**	Wiener-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
630	**WiA_Dz(p)**	average Wiener-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
631	**AVS_Dz(p)**	average vertex sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors
632	**H_Dz(p)**	Harary-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
633	**Chi_Dz(p)**	Randic-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
634	**ChiA_Dz(p)**	average Randic-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
635	**J_Dz(p)**	Balaban-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors

No.	Name	Description	Block
636	**HyWi_Dz(p)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
637	**SpAbs_Dz(p)**	graph energy from Barysz matrix weighted by polarizability	2D matrix-based descriptors
638	**SpPos_Dz(p)**	spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors
639	**SpPosA_Dz(p)**	normalized spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors
640	**SpPosLog_Dz(p)**	logarithmic spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors
641	**SpMax_Dz(p)**	leading eigenvalue from Barysz matrix weighted by polarizability	2D matrix-based descriptors
642	**SpMaxA_Dz(p)**	normalized leading eigenvalue from Barysz matrix weighted by polarizability	2D matrix-based descriptors
643	**SpDiam_Dz(p)**	spectral diameter from Barysz matrix weighted by polarizability	2D matrix-based descriptors
644	**SpAD_Dz(p)**	spectral absolute deviation from Barysz matrix weighted by polarizability	2D matrix-based descriptors
645	**SpMAD_Dz(p)**	spectral mean absolute deviation from Barysz matrix weighted by polarizability	2D matrix-based descriptors
646	**Ho_Dz(p)**	Hosoya-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
647	**EE_Dz(p)**	Estrada-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
648	**SM1_Dz(p)**	spectral moment of order 1 from Barysz matrix weighted by polarizability	2D matrix-based descriptors
649	**SM2_Dz(p)**	spectral moment of order 2 from Barysz matrix weighted by polarizability	2D matrix-based descriptors

No.	Name	Description	Block
650	**SM3_Dz(p)**	spectral moment of order 3 from Barysz matrix weighted by polarizability	2D matrix-based descriptors
651	**SM4_Dz(p)**	spectral moment of order 4 from Barysz matrix weighted by polarizability	2D matrix-based descriptors
652	**SM5_Dz(p)**	spectral moment of order 5 from Barysz matrix weighted by polarizability	2D matrix-based descriptors
653	**SM6_Dz(p)**	spectral moment of order 6 from Barysz matrix weighted by polarizability	2D matrix-based descriptors
654	**VE1_Dz(p)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
655	**VE2_Dz(p)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
656	**VE3_Dz(p)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors
657	**VE1sign_Dz(p)**	coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors
658	**VE2sign_Dz(p)**	average coefficient of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors
659	**VE3sign_Dz(p)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors
660	**VR1_Dz(p)**	Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
661	**VR2_Dz(p)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
662	**VR3_Dz(p)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
663	**Wi_Dz(i)**	Wiener-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
664	**WiA_Dz(i)**	average Wiener-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
665	**AVS_Dz(i)**	average vertex sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
666	**H_Dz(i)**	Harary-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
667	**Chi_Dz(i)**	Randic-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
668	**ChiA_Dz(i)**	average Randic-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
669	**J_Dz(i)**	Balaban-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
670	**HyWi_Dz(i)**	hyper-Wiener-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
671	**SpAbs_Dz(i)**	graph energy from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
672	**SpPos_Dz(i)**	spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
673	**SpPosA_Dz(i)**	normalized spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
674	**SpPosLog_Dz(i)**	logarithmic spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
675	**SpMax_Dz(i)**	leading eigenvalue from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
676	**SpMaxA_Dz(i)**	normalized leading eigenvalue from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
677	**SpDiam_Dz(i)**	spectral diameter from Barysz matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
678	**SpAD_Dz(i)**	spectral absolute deviation from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
679	**SpMAD_Dz(i)**	spectral mean absolute deviation from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
680	**Ho_Dz(i)**	Hosoya-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
681	**EE_Dz(i)**	Estrada-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
682	**SM1_Dz(i)**	spectral moment of order 1 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
683	**SM2_Dz(i)**	spectral moment of order 2 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
684	**SM3_Dz(i)**	spectral moment of order 3 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
685	**SM4_Dz(i)**	spectral moment of order 4 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
686	**SM5_Dz(i)**	spectral moment of order 5 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
687	**SM6_Dz(i)**	spectral moment of order 6 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
688	**VE1_Dz(i)**	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
689	**VE2_Dz(i)**	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
690	**VE3_Dz(i)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
691	**VE1sign_Dz(i)**	coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
692	**VE2sign_Dz(i)**	average coefficient of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
693	**VE3sign_Dz(i)**	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
694	**VR1_Dz(i)**	Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
695	**VR2_Dz(i)**	normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
696	**VR3_Dz(i)**	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors
697	**Wi_B(m)**	Wiener-like index from Burden matrix weighted by mass	2D matrix-based descriptors
698	**WiA_B(m)**	average Wiener-like index from Burden matrix weighted by mass	2D matrix-based descriptors
699	**AVS_B(m)**	average vertex sum from Burden matrix weighted by mass	2D matrix-based descriptors
700	**Chi_B(m)**	Randic-like index from Burden matrix weighted by mass	2D matrix-based descriptors
701	**ChiA_B(m)**	average Randic-like index from Burden matrix weighted by mass	2D matrix-based descriptors
702	**J_B(m)**	Balaban-like index from Burden matrix weighted by mass	2D matrix-based descriptors
703	**HyWi_B(m)**	hyper-Wiener-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors
704	**SpAbs_B(m)**	graph energy from Burden matrix weighted by mass	2D matrix-based descriptors
705	**SpPos_B(m)**	spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors

No.	Name	Description	Block
706	**SpPosA_B(m)**	normalized spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors
707	**SpPosLog_B(m)**	logarithmic spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors
708	**SpMax_B(m)**	leading eigenvalue from Burden matrix weighted by mass	2D matrix-based descriptors
709	**SpMaxA_B(m)**	normalized leading eigenvalue from Burden matrix weighted by mass	2D matrix-based descriptors
710	**SpDiam_B(m)**	spectral diameter from Burden matrix weighted by mass	2D matrix-based descriptors
711	**SpAD_B(m)**	spectral absolute deviation from Burden matrix weighted by mass	2D matrix-based descriptors
712	**SpMAD_B(m)**	spectral mean absolute deviation from Burden matrix weighted by mass	2D matrix-based descriptors
713	**Ho_B(m)**	Hosoya-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors
714	**EE_B(m)**	Estrada-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors
715	**SM1_B(m)**	spectral moment of order 1 from Burden matrix weighted by mass	2D matrix-based descriptors
716	**SM2_B(m)**	spectral moment of order 2 from Burden matrix weighted by mass	2D matrix-based descriptors
717	**SM3_B(m)**	spectral moment of order 3 from Burden matrix weighted by mass	2D matrix-based descriptors
718	**SM4_B(m)**	spectral moment of order 4 from Burden matrix weighted by mass	2D matrix-based descriptors
719	**SM5_B(m)**	spectral moment of order 5 from Burden matrix weighted by mass	2D matrix-based descriptors

No.	Name	Description	Block
720	**SM6_B(m)**	spectral moment of order 6 from Burden matrix weighted by mass	2D matrix-based descriptors
721	**VE1_B(m)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors
722	**VE2_B(m)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors
723	**VE3_B(m)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors
724	**VE1sign_B(m)**	coefficient sum of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors
725	**VE2sign_B(m)**	average coefficient of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors
726	**VE3sign_B(m)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors
727	**VR1_B(m)**	Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors
728	**VR2_B(m)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors
729	**VR3_B(m)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors
730	**Wi_B(v)**	Wiener-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
731	**WiA_B(v)**	average Wiener-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
732	**AVS_B(v)**	average vertex sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
733	**Chi_B(v)**	Randic-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
734	**ChiA_B(v)**	average Randic-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
735	**J_B(v)**	Balaban-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
736	**HyWi_B(v)**	hyper-Wiener-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
737	**SpAbs_B(v)**	graph energy from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
738	**SpPos_B(v)**	spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
739	**SpPosA_B(v)**	normalized spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
740	**SpPosLog_B(v)**	logarithmic spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
741	**SpMax_B(v)**	leading eigenvalue from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
742	**SpMaxA_B(v)**	normalized leading eigenvalue from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
743	**SpDiam_B(v)**	spectral diameter from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
744	**SpAD_B(v)**	spectral absolute deviation from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
745	**SpMAD_B(v)**	spectral mean absolute deviation from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
746	**Ho_B(v)**	Hosoya-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
747	**EE_B(v)**	Estrada-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
748	**SM1_B(v)**	spectral moment of order 1 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
749	**SM2_B(v)**	spectral moment of order 2 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
750	**SM3_B(v)**	spectral moment of order 3 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
751	**SM4_B(v)**	spectral moment of order 4 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
752	**SM5_B(v)**	spectral moment of order 5 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
753	**SM6_B(v)**	spectral moment of order 6 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
754	**VE1_B(v)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
755	**VE2_B(v)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
756	**VE3_B(v)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
757	**VE1sign_B(v)**	coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
758	**VE2sign_B(v)**	average coefficient of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
759	**VE3sign_B(v)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
760	**VR1_B(v)**	Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
761	**VR2_B(v)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors

No.	Name	Description	Block
762	**VR3_B(v)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors
763	**Wi_B(e)**	Wiener-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
764	**WiA_B(e)**	average Wiener-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
765	**AVS_B(e)**	average vertex sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
766	**Chi_B(e)**	Randic-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
767	**ChiA_B(e)**	average Randic-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
768	**J_B(e)**	Balaban-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
769	**HyWi_B(e)**	hyper-Wiener-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
770	**SpAbs_B(e)**	graph energy from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
771	**SpPos_B(e)**	spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
772	**SpPosA_B(e)**	normalized spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
773	**SpPosLog_B(e)**	logarithmic spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
774	**SpMax_B(e)**	leading eigenvalue from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
775	**SpMaxA_B(e)**	normalized leading eigenvalue from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors

No.	Name	Description	Block
776	**SpDiam_B(e)**	spectral diameter from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
777	**SpAD_B(e)**	spectral absolute deviation from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
778	**SpMAD_B(e)**	spectral mean absolute deviation from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
779	**Ho_B(e)**	Hosoya-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
780	**EE_B(e)**	Estrada-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
781	**SM1_B(e)**	spectral moment of order 1 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
782	**SM2_B(e)**	spectral moment of order 2 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
783	**SM3_B(e)**	spectral moment of order 3 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
784	**SM4_B(e)**	spectral moment of order 4 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
785	**SM5_B(e)**	spectral moment of order 5 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
786	**SM6_B(e)**	spectral moment of order 6 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
787	**VE1_B(e)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
788	**VE2_B(e)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
789	**VE3_B(e)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors

No.	Name	Description	Block
790	**VE1sign_B(e)**	coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
791	**VE2sign_B(e)**	average coefficient of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
792	**VE3sign_B(e)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
793	**VR1_B(e)**	Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
794	**VR2_B(e)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
795	**VR3_B(e)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors
796	**Wi_B(p)**	Wiener-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors
797	**WiA_B(p)**	average Wiener-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors
798	**AVS_B(p)**	average vertex sum from Burden matrix weighted by polarizability	2D matrix-based descriptors
799	**Chi_B(p)**	Randic-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors
800	**ChiA_B(p)**	average Randic-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors
801	**J_B(p)**	Balaban-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors
802	**HyWi_B(p)**	hyper-Wiener-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors
803	**SpAbs_B(p)**	graph energy from Burden matrix weighted by polarizability	2D matrix-based descriptors

No.	Name	Description	Block
804	**SpPos_B(p)**	spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors
805	**SpPosA_B(p)**	normalized spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors
806	**SpPosLog_B(p)**	logarithmic spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors
807	**SpMax_B(p)**	leading eigenvalue from Burden matrix weighted by polarizability	2D matrix-based descriptors
808	**SpMaxA_B(p)**	normalized leading eigenvalue from Burden matrix weighted by polarizability	2D matrix-based descriptors
809	**SpDiam_B(p)**	spectral diameter from Burden matrix weighted by polarizability	2D matrix-based descriptors
810	**SpAD_B(p)**	spectral absolute deviation from Burden matrix weighted by polarizability	2D matrix-based descriptors
811	**SpMAD_B(p)**	spectral mean absolute deviation from Burden matrix weighted by polarizability	2D matrix-based descriptors
812	**Ho_B(p)**	Hosoya-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors
813	**EE_B(p)**	Estrada-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors
814	**SM1_B(p)**	spectral moment of order 1 from Burden matrix weighted by polarizability	2D matrix-based descriptors
815	**SM2_B(p)**	spectral moment of order 2 from Burden matrix weighted by polarizability	2D matrix-based descriptors
816	**SM3_B(p)**	spectral moment of order 3 from Burden matrix weighted by polarizability	2D matrix-based descriptors
817	**SM4_B(p)**	spectral moment of order 4 from Burden matrix weighted by polarizability	2D matrix-based descriptors

No.	Name	Description	Block
818	**SM5_B(p)**	spectral moment of order 5 from Burden matrix weighted by polarizability	2D matrix-based descriptors
819	**SM6_B(p)**	spectral moment of order 6 from Burden matrix weighted by polarizability	2D matrix-based descriptors
820	**VE1_B(p)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors
821	**VE2_B(p)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors
822	**VE3_B(p)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors
823	**VE1sign_B(p)**	coefficient sum of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors
824	**VE2sign_B(p)**	average coefficient of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors
825	**VE3sign_B(p)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors
826	**VR1_B(p)**	Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors
827	**VR2_B(p)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors
828	**VR3_B(p)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors
829	**Wi_B(i)**	Wiener-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
830	**WiA_B(i)**	average Wiener-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
831	**AVS_B(i)**	average vertex sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
832	**Chi_B(i)**	Randic-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
833	**ChiA_B(i)**	average Randic-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
834	**J_B(i)**	Balaban-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
835	**HyWi_B(i)**	hyper-Wiener-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors
836	**SpAbs_B(i)**	graph energy from Burden matrix weighted by ionization potential	2D matrix-based descriptors
837	**SpPos_B(i)**	spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors
838	**SpPosA_B(i)**	normalized spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors
839	**SpPosLog_B(i)**	logarithmic spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors
840	**SpMax_B(i)**	leading eigenvalue from Burden matrix weighted by ionization potential	2D matrix-based descriptors
841	**SpMaxA_B(i)**	normalized leading eigenvalue from Burden matrix weighted by ionization potential	2D matrix-based descriptors
842	**SpDiam_B(i)**	spectral diameter from Burden matrix weighted by ionization potential	2D matrix-based descriptors
843	**SpAD_B(i)**	spectral absolute deviation from Burden matrix weighted by ionization potential	2D matrix-based descriptors
844	**SpMAD_B(i)**	spectral mean absolute deviation from Burden matrix weighted by ionization potential	2D matrix-based descriptors
845	**Ho_B(i)**	Hosoya-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
846	**EE_B(i)**	Estrada-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors
847	**SM1_B(i)**	spectral moment of order 1 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
848	**SM2_B(i)**	spectral moment of order 2 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
849	**SM3_B(i)**	spectral moment of order 3 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
850	**SM4_B(i)**	spectral moment of order 4 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
851	**SM5_B(i)**	spectral moment of order 5 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
852	**SM6_B(i)**	spectral moment of order 6 from Burden matrix weighted by ionization potential	2D matrix-based descriptors
853	**VE1_B(i)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors
854	**VE2_B(i)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors
855	**VE3_B(i)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors
856	**VE1sign_B(i)**	coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors
857	**VE2sign_B(i)**	average coefficient of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors
858	**VE3sign_B(i)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors
859	**VR1_B(i)**	Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors

No.	Name	Description	Block
860	**VR2_B(i)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
861	**VR3_B(i)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors
862	**Wi_B(s)**	Wiener-like index from Burden matrix weighted by I-State	2D matrix-based descriptors
863	**WiA_B(s)**	average Wiener-like index from Burden matrix weighted by I-State	2D matrix-based descriptors
864	**AVS_B(s)**	average vertex sum from Burden matrix weighted by I-State	2D matrix-based descriptors
865	**Chi_B(s)**	Randic-like index from Burden matrix weighted by I-State	2D matrix-based descriptors
866	**ChiA_B(s)**	average Randic-like index from Burden matrix weighted by I-State	2D matrix-based descriptors
867	**J_B(s)**	Balaban-like index from Burden matrix weighted by I-State	2D matrix-based descriptors
868	**HyWi_B(s)**	hyper-Wiener-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors
869	**SpAbs_B(s)**	graph energy from Burden matrix weighted by I-State	2D matrix-based descriptors
870	**SpPos_B(s)**	spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors
871	**SpPosA_B(s)**	normalized spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors
872	**SpPosLog_B(s)**	logarithmic spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors
873	**SpMax_B(s)**	leading eigenvalue from Burden matrix weighted by I-State	2D matrix-based descriptors

No.	Name	Description	Block
874	**SpMaxA_B(s)**	normalized leading eigenvalue from Burden matrix weighted by I-State	2D matrix-based descriptors
875	**SpDiam_B(s)**	spectral diameter from Burden matrix weighted by I-State	2D matrix-based descriptors
876	**SpAD_B(s)**	spectral absolute deviation from Burden matrix weighted by I-State	2D matrix-based descriptors
877	**SpMAD_B(s)**	spectral mean absolute deviation from Burden matrix weighted by I-State	2D matrix-based descriptors
878	**Ho_B(s)**	Hosoya-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors
879	**EE_B(s)**	Estrada-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors
880	**SM1_B(s)**	spectral moment of order 1 from Burden matrix weighted by I-State	2D matrix-based descriptors
881	**SM2_B(s)**	spectral moment of order 2 from Burden matrix weighted by I-State	2D matrix-based descriptors
882	**SM3_B(s)**	spectral moment of order 3 from Burden matrix weighted by I-State	2D matrix-based descriptors
883	**SM4_B(s)**	spectral moment of order 4 from Burden matrix weighted by I-State	2D matrix-based descriptors
884	**SM5_B(s)**	spectral moment of order 5 from Burden matrix weighted by I-State	2D matrix-based descriptors
885	**SM6_B(s)**	spectral moment of order 6 from Burden matrix weighted by I-State	2D matrix-based descriptors
886	**VE1_B(s)**	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors
887	**VE2_B(s)**	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors

No.	Name	Description	Block
888	**VE3_B(s)**	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors
889	**VE1sign_B(s)**	coefficient sum of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors
890	**VE2sign_B(s)**	average coefficient of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors
891	**VE3sign_B(s)**	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors
892	**VR1_B(s)**	Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors
893	**VR2_B(s)**	normalized Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors
894	**VR3_B(s)**	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors
895	**ATS1m**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by mass	2D autocorrelations
896	**ATS2m**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by mass	2D autocorrelations
897	**ATS3m**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by mass	2D autocorrelations
898	**ATS4m**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by mass	2D autocorrelations
899	**ATS5m**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by mass	2D autocorrelations
900	**ATS6m**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by mass	2D autocorrelations
901	**ATS7m**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by mass	2D autocorrelations
902	**ATS8m**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by mass	2D autocorrelations
903	**ATS1v**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by van der Waals volume	2D autocorrelations
904	**ATS2v**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by van der Waals volume	2D autocorrelations

No.	Name	Description	Block
905	**ATS3v**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by van der Waals volume	2D autocorrelations
906	**ATS4v**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by van der Waals volume	2D autocorrelations
907	**ATS5v**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by van der Waals volume	2D autocorrelations
908	**ATS6v**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by van der Waals volume	2D autocorrelations
909	**ATS7v**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by van der Waals volume	2D autocorrelations
910	**ATS8v**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume	2D autocorrelations
911	**ATS1e**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by Sanderson electronegativity	2D autocorrelations
912	**ATS2e**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by Sanderson electronegativity	2D autocorrelations
913	**ATS3e**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by Sanderson electronegativity	2D autocorrelations
914	**ATS4e**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by Sanderson electronegativity	2D autocorrelations
915	**ATS5e**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by Sanderson electronegativity	2D autocorrelations
916	**ATS6e**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by Sanderson electronegativity	2D autocorrelations
917	**ATS7e**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by Sanderson electronegativity	2D autocorrelations
918	**ATS8e**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by Sanderson electronegativity	2D autocorrelations
919	**ATS1p**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by polarizability	2D autocorrelations
920	**ATS2p**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by polarizability	2D autocorrelations
921	**ATS3p**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability	2D autocorrelations
922	**ATS4p**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by polarizability	2D autocorrelations
923	**ATS5p**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by polarizability	2D autocorrelations

No.	Name	Description	Block
924	**ATS6p**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by polarizability	2D autocorrelations
925	**ATS7p**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by polarizability	2D autocorrelations
926	**ATS8p**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by polarizability	2D autocorrelations
927	**ATS1i**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by ionization potential	2D autocorrelations
928	**ATS2i**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by ionization potential	2D autocorrelations
929	**ATS3i**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by ionization potential	2D autocorrelations
930	**ATS4i**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by ionization potential	2D autocorrelations
931	**ATS5i**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by ionization potential	2D autocorrelations
932	**ATS6i**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by ionization potential	2D autocorrelations
933	**ATS7i**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by ionization potential	2D autocorrelations
934	**ATS8i**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by ionization potential	2D autocorrelations
935	**ATS1s**	Broto-Moreau autocorrelation of lag 1 (log function) weighted by I-state	2D autocorrelations
936	**ATS2s**	Broto-Moreau autocorrelation of lag 2 (log function) weighted by I-state	2D autocorrelations
937	**ATS3s**	Broto-Moreau autocorrelation of lag 3 (log function) weighted by I-state	2D autocorrelations
938	**ATS4s**	Broto-Moreau autocorrelation of lag 4 (log function) weighted by I-state	2D autocorrelations
939	**ATS5s**	Broto-Moreau autocorrelation of lag 5 (log function) weighted by I-state	2D autocorrelations
940	**ATS6s**	Broto-Moreau autocorrelation of lag 6 (log function) weighted by I-state	2D autocorrelations
941	**ATS7s**	Broto-Moreau autocorrelation of lag 7 (log function) weighted by I-state	2D autocorrelations
942	**ATS8s**	Broto-Moreau autocorrelation of lag 8 (log function) weighted by I-state	2D autocorrelations

No.	Name	Description	Block
943	**ATSC1m**	Centred Broto-Moreau autocorrelation of lag 1 weighted by mass	2D autocorrelations
944	**ATSC2m**	Centred Broto-Moreau autocorrelation of lag 2 weighted by mass	2D autocorrelations
945	**ATSC3m**	Centred Broto-Moreau autocorrelation of lag 3 weighted by mass	2D autocorrelations
946	**ATSC4m**	Centred Broto-Moreau autocorrelation of lag 4 weighted by mass	2D autocorrelations
947	**ATSC5m**	Centred Broto-Moreau autocorrelation of lag 5 weighted by mass	2D autocorrelations
948	**ATSC6m**	Centred Broto-Moreau autocorrelation of lag 6 weighted by mass	2D autocorrelations
949	**ATSC7m**	Centred Broto-Moreau autocorrelation of lag 7 weighted by mass	2D autocorrelations
950	**ATSC8m**	Centred Broto-Moreau autocorrelation of lag 8 weighted by mass	2D autocorrelations
951	**ATSC1v**	Centred Broto-Moreau autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations
952	**ATSC2v**	Centred Broto-Moreau autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
953	**ATSC3v**	Centred Broto-Moreau autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
954	**ATSC4v**	Centred Broto-Moreau autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
955	**ATSC5v**	Centred Broto-Moreau autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
956	**ATSC6v**	Centred Broto-Moreau autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
957	**ATSC7v**	Centred Broto-Moreau autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
958	**ATSC8v**	Centred Broto-Moreau autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
959	**ATSC1e**	Centred Broto-Moreau autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
960	**ATSC2e**	Centred Broto-Moreau autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations
961	**ATSC3e**	Centred Broto-Moreau autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations

No.	Name	Description	Block
962	**ATSC4e**	Centred Broto-Moreau autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
963	**ATSC5e**	Centred Broto-Moreau autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
964	**ATSC6e**	Centred Broto-Moreau autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
965	**ATSC7e**	Centred Broto-Moreau autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
966	**ATSC8e**	Centred Broto-Moreau autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
967	**ATSC1p**	Centred Broto-Moreau autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
968	**ATSC2p**	Centred Broto-Moreau autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
969	**ATSC3p**	Centred Broto-Moreau autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
970	**ATSC4p**	Centred Broto-Moreau autocorrelation of lag 4 weighted by polarizability	2D autocorrelations
971	**ATSC5p**	Centred Broto-Moreau autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
972	**ATSC6p**	Centred Broto-Moreau autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
973	**ATSC7p**	Centred Broto-Moreau autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
974	**ATSC8p**	Centred Broto-Moreau autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
975	**ATSC1i**	Centred Broto-Moreau autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
976	**ATSC2i**	Centred Broto-Moreau autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
977	**ATSC3i**	Centred Broto-Moreau autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations
978	**ATSC4i**	Centred Broto-Moreau autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations
979	**ATSC5i**	Centred Broto-Moreau autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations
980	**ATSC6i**	Centred Broto-Moreau autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations

No.	Name	Description	Block
981	**ATSC7i**	Centred Broto-Moreau autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
982	**ATSC8i**	Centred Broto-Moreau autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
983	**ATSC1s**	Centred Broto-Moreau autocorrelation of lag 1 weighted by I-state	2D autocorrelations
984	**ATSC2s**	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state	2D autocorrelations
985	**ATSC3s**	Centred Broto-Moreau autocorrelation of lag 3 weighted by I-state	2D autocorrelations
986	**ATSC4s**	Centred Broto-Moreau autocorrelation of lag 4 weighted by I-state	2D autocorrelations
987	**ATSC5s**	Centred Broto-Moreau autocorrelation of lag 5 weighted by I-state	2D autocorrelations
988	**ATSC6s**	Centred Broto-Moreau autocorrelation of lag 6 weighted by I-state	2D autocorrelations
989	**ATSC7s**	Centred Broto-Moreau autocorrelation of lag 7 weighted by I-state	2D autocorrelations
990	**ATSC8s**	Centred Broto-Moreau autocorrelation of lag 8 weighted by I-state	2D autocorrelations
991	**MATS1m**	Moran autocorrelation of lag 1 weighted by mass	2D autocorrelations
992	**MATS2m**	Moran autocorrelation of lag 2 weighted by mass	2D autocorrelations
993	**MATS3m**	Moran autocorrelation of lag 3 weighted by mass	2D autocorrelations
994	**MATS4m**	Moran autocorrelation of lag 4 weighted by mass	2D autocorrelations
995	**MATS5m**	Moran autocorrelation of lag 5 weighted by mass	2D autocorrelations
996	**MATS6m**	Moran autocorrelation of lag 6 weighted by mass	2D autocorrelations
997	**MATS7m**	Moran autocorrelation of lag 7 weighted by mass	2D autocorrelations
998	**MATS8m**	Moran autocorrelation of lag 8 weighted by mass	2D autocorrelations
999	**MATS1v**	Moran autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations

No.	Name	Description	Block
1000	**MATS2v**	Moran autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
1001	**MATS3v**	Moran autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
1002	**MATS4v**	Moran autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
1003	**MATS5v**	Moran autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
1004	**MATS6v**	Moran autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
1005	**MATS7v**	Moran autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
1006	**MATS8v**	Moran autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
1007	**MATS1e**	Moran autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
1008	**MATS2e**	Moran autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations
1009	**MATS3e**	Moran autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations
1010	**MATS4e**	Moran autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
1011	**MATS5e**	Moran autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
1012	**MATS6e**	Moran autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
1013	**MATS7e**	Moran autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
1014	**MATS8e**	Moran autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
1015	**MATS1p**	Moran autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
1016	**MATS2p**	Moran autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
1017	**MATS3p**	Moran autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
1018	**MATS4p**	Moran autocorrelation of lag 4 weighted by polarizability	2D autocorrelations

No.	Name	Description	Block
1019	**MATS5p**	Moran autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
1020	**MATS6p**	Moran autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
1021	**MATS7p**	Moran autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
1022	**MATS8p**	Moran autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
1023	**MATS1i**	Moran autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
1024	**MATS2i**	Moran autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
1025	**MATS3i**	Moran autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations
1026	**MATS4i**	Moran autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations
1027	**MATS5i**	Moran autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations
1028	**MATS6i**	Moran autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations
1029	**MATS7i**	Moran autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
1030	**MATS8i**	Moran autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
1031	**MATS1s**	Moran autocorrelation of lag 1 weighted by I-state	2D autocorrelations
1032	**MATS2s**	Moran autocorrelation of lag 2 weighted by I-state	2D autocorrelations
1033	**MATS3s**	Moran autocorrelation of lag 3 weighted by I-state	2D autocorrelations
1034	**MATS4s**	Moran autocorrelation of lag 4 weighted by I-state	2D autocorrelations
1035	**MATS5s**	Moran autocorrelation of lag 5 weighted by I-state	2D autocorrelations
1036	**MATS6s**	Moran autocorrelation of lag 6 weighted by I-state	2D autocorrelations
1037	**MATS7s**	Moran autocorrelation of lag 7 weighted by I-state	2D autocorrelations

No.	Name	Description	Block
1038	**MATS8s**	Moran autocorrelation of lag 8 weighted by I-state	2D autocorrelations
1039	**GATS1m**	Geary autocorrelation of lag 1 weighted by mass	2D autocorrelations
1040	**GATS2m**	Geary autocorrelation of lag 2 weighted by mass	2D autocorrelations
1041	**GATS3m**	Geary autocorrelation of lag 3 weighted by mass	2D autocorrelations
1042	**GATS4m**	Geary autocorrelation of lag 4 weighted by mass	2D autocorrelations
1043	**GATS5m**	Geary autocorrelation of lag 5 weighted by mass	2D autocorrelations
1044	**GATS6m**	Geary autocorrelation of lag 6 weighted by mass	2D autocorrelations
1045	**GATS7m**	Geary autocorrelation of lag 7 weighted by mass	2D autocorrelations
1046	**GATS8m**	Geary autocorrelation of lag 8 weighted by mass	2D autocorrelations
1047	**GATS1v**	Geary autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations
1048	**GATS2v**	Geary autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
1049	**GATS3v**	Geary autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
1050	**GATS4v**	Geary autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
1051	**GATS5v**	Geary autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
1052	**GATS6v**	Geary autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
1053	**GATS7v**	Geary autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
1054	**GATS8v**	Geary autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
1055	**GATS1e**	Geary autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
1056	**GATS2e**	Geary autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations

No.	Name	Description	Block
1057	**GATS3e**	Geary autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations
1058	**GATS4e**	Geary autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
1059	**GATS5e**	Geary autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
1060	**GATS6e**	Geary autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
1061	**GATS7e**	Geary autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
1062	**GATS8e**	Geary autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
1063	**GATS1p**	Geary autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
1064	**GATS2p**	Geary autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
1065	**GATS3p**	Geary autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
1066	**GATS4p**	Geary autocorrelation of lag 4 weighted by polarizability	2D autocorrelations
1067	**GATS5p**	Geary autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
1068	**GATS6p**	Geary autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
1069	**GATS7p**	Geary autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
1070	**GATS8p**	Geary autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
1071	**GATS1i**	Geary autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
1072	**GATS2i**	Geary autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
1073	**GATS3i**	Geary autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations
1074	**GATS4i**	Geary autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations
1075	**GATS5i**	Geary autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations

No.	Name	Description	Block
1076	**GATS6i**	Geary autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations
1077	**GATS7i**	Geary autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
1078	**GATS8i**	Geary autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
1079	**GATS1s**	Geary autocorrelation of lag 1 weighted by I-state	2D autocorrelations
1080	**GATS2s**	Geary autocorrelation of lag 2 weighted by I-state	2D autocorrelations
1081	**GATS3s**	Geary autocorrelation of lag 3 weighted by I-state	2D autocorrelations
1082	**GATS4s**	Geary autocorrelation of lag 4 weighted by I-state	2D autocorrelations
1083	**GATS5s**	Geary autocorrelation of lag 5 weighted by I-state	2D autocorrelations
1084	**GATS6s**	Geary autocorrelation of lag 6 weighted by I-state	2D autocorrelations
1085	**GATS7s**	Geary autocorrelation of lag 7 weighted by I-state	2D autocorrelations
1086	**GATS8s**	Geary autocorrelation of lag 8 weighted by I-state	2D autocorrelations
1087	**GGI1**	topological charge index of order 1	2D autocorrelations
1088	**GGI2**	topological charge index of order 2	2D autocorrelations
1089	**GGI3**	topological charge index of order 3	2D autocorrelations
1090	**GGI4**	topological charge index of order 4	2D autocorrelations
1091	**GGI5**	topological charge index of order 5	2D autocorrelations
1092	**GGI6**	topological charge index of order 6	2D autocorrelations
1093	**GGI7**	topological charge index of order 7	2D autocorrelations
1094	**GGI8**	topological charge index of order 8	2D autocorrelations

No.	Name	Description	Block
1095	**GGI9**	topological charge index of order 9	2D autocorrelations
1096	**GGI10**	topological charge index of order 10	2D autocorrelations
1097	**JGI1**	mean topological charge index of order 1	2D autocorrelations
1098	**JGI2**	mean topological charge index of order 2	2D autocorrelations
1099	**JGI3**	mean topological charge index of order 3	2D autocorrelations
1100	**JGI4**	mean topological charge index of order 4	2D autocorrelations
1101	**JGI5**	mean topological charge index of order 5	2D autocorrelations
1102	**JGI6**	mean topological charge index of order 6	2D autocorrelations
1103	**JGI7**	mean topological charge index of order 7	2D autocorrelations
1104	**JGI8**	mean topological charge index of order 8	2D autocorrelations
1105	**JGI9**	mean topological charge index of order 9	2D autocorrelations
1106	**JGI10**	mean topological charge index of order 10	2D autocorrelations
1107	**JGT**	global topological charge index	2D autocorrelations
1108	**SpMax1_Bh(m)**	largest eigenvalue n. 1 of Burden matrix weighted by mass	Burden eigenvalues
1109	**SpMax2_Bh(m)**	largest eigenvalue n. 2 of Burden matrix weighted by mass	Burden eigenvalues
1110	**SpMax3_Bh(m)**	largest eigenvalue n. 3 of Burden matrix weighted by mass	Burden eigenvalues
1111	**SpMax4_Bh(m)**	largest eigenvalue n. 4 of Burden matrix weighted by mass	Burden eigenvalues
1112	**SpMax5_Bh(m)**	largest eigenvalue n. 5 of Burden matrix weighted by mass	Burden eigenvalues
1113	**SpMax6_Bh(m)**	largest eigenvalue n. 6 of Burden matrix weighted by mass	Burden eigenvalues

No.	Name	Description	Block
1114	**SpMax7_Bh(m)**	largest eigenvalue n. 7 of Burden matrix weighted by mass	Burden eigenvalues
1115	**SpMax8_Bh(m)**	largest eigenvalue n. 8 of Burden matrix weighted by mass	Burden eigenvalues
1116	**SpMax1_Bh(v)**	largest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1117	**SpMax2_Bh(v)**	largest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1118	**SpMax3_Bh(v)**	largest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1119	**SpMax4_Bh(v)**	largest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1120	**SpMax5_Bh(v)**	largest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1121	**SpMax6_Bh(v)**	largest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1122	**SpMax7_Bh(v)**	largest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1123	**SpMax8_Bh(v)**	largest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1124	**SpMax1_Bh(e)**	largest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1125	**SpMax2_Bh(e)**	largest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1126	**SpMax3_Bh(e)**	largest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1127	**SpMax4_Bh(e)**	largest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1128	**SpMax5_Bh(e)**	largest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1129	**SpMax6_Bh(e)**	largest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1130	**SpMax7_Bh(e)**	largest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1131	**SpMax8_Bh(e)**	largest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1132	**SpMax1_Bh(p)**	largest eigenvalue n. 1 of Burden matrix weighted by polarizability	Burden eigenvalues

No.	Name	Description	Block
1133	**SpMax2_Bh(p)**	largest eigenvalue n. 2 of Burden matrix weighted by polarizability	Burden eigenvalues
1134	**SpMax3_Bh(p)**	largest eigenvalue n. 3 of Burden matrix weighted by polarizability	Burden eigenvalues
1135	**SpMax4_Bh(p)**	largest eigenvalue n. 4 of Burden matrix weighted by polarizability	Burden eigenvalues
1136	**SpMax5_Bh(p)**	largest eigenvalue n. 5 of Burden matrix weighted by polarizability	Burden eigenvalues
1137	**SpMax6_Bh(p)**	largest eigenvalue n. 6 of Burden matrix weighted by polarizability	Burden eigenvalues
1138	**SpMax7_Bh(p)**	largest eigenvalue n. 7 of Burden matrix weighted by polarizability	Burden eigenvalues
1139	**SpMax8_Bh(p)**	largest eigenvalue n. 8 of Burden matrix weighted by polarizability	Burden eigenvalues
1140	**SpMax1_Bh(i)**	largest eigenvalue n. 1 of Burden matrix weighted by ionization potential	Burden eigenvalues
1141	**SpMax2_Bh(i)**	largest eigenvalue n. 2 of Burden matrix weighted by ionization potential	Burden eigenvalues
1142	**SpMax3_Bh(i)**	largest eigenvalue n. 3 of Burden matrix weighted by ionization potential	Burden eigenvalues
1143	**SpMax4_Bh(i)**	largest eigenvalue n. 4 of Burden matrix weighted by ionization potential	Burden eigenvalues
1144	**SpMax5_Bh(i)**	largest eigenvalue n. 5 of Burden matrix weighted by ionization potential	Burden eigenvalues
1145	**SpMax6_Bh(i)**	largest eigenvalue n. 6 of Burden matrix weighted by ionization potential	Burden eigenvalues
1146	**SpMax7_Bh(i)**	largest eigenvalue n. 7 of Burden matrix weighted by ionization potential	Burden eigenvalues
1147	**SpMax8_Bh(i)**	largest eigenvalue n. 8 of Burden matrix weighted by ionization potential	Burden eigenvalues
1148	**SpMax1_Bh(s)**	largest eigenvalue n. 1 of Burden matrix weighted by I-state	Burden eigenvalues
1149	**SpMax2_Bh(s)**	largest eigenvalue n. 2 of Burden matrix weighted by I-state	Burden eigenvalues
1150	**SpMax3_Bh(s)**	largest eigenvalue n. 3 of Burden matrix weighted by I-state	Burden eigenvalues
1151	**SpMax4_Bh(s)**	largest eigenvalue n. 4 of Burden matrix weighted by I-state	Burden eigenvalues

No.	Name	Description	Block
1152	**SpMax5_Bh(s)**	largest eigenvalue n. 5 of Burden matrix weighted by I-state	Burden eigenvalues
1153	**SpMax6_Bh(s)**	largest eigenvalue n. 6 of Burden matrix weighted by I-state	Burden eigenvalues
1154	**SpMax7_Bh(s)**	largest eigenvalue n. 7 of Burden matrix weighted by I-state	Burden eigenvalues
1155	**SpMax8_Bh(s)**	largest eigenvalue n. 8 of Burden matrix weighted by I-state	Burden eigenvalues
1156	**SpMin1_Bh(m)**	smallest eigenvalue n. 1 of Burden matrix weighted by mass	Burden eigenvalues
1157	**SpMin2_Bh(m)**	smallest eigenvalue n. 2 of Burden matrix weighted by mass	Burden eigenvalues
1158	**SpMin3_Bh(m)**	smallest eigenvalue n. 3 of Burden matrix weighted by mass	Burden eigenvalues
1159	**SpMin4_Bh(m)**	smallest eigenvalue n. 4 of Burden matrix weighted by mass	Burden eigenvalues
1160	**SpMin5_Bh(m)**	smallest eigenvalue n. 5 of Burden matrix weighted by mass	Burden eigenvalues
1161	**SpMin6_Bh(m)**	smallest eigenvalue n. 6 of Burden matrix weighted by mass	Burden eigenvalues
1162	**SpMin7_Bh(m)**	smallest eigenvalue n. 7 of Burden matrix weighted by mass	Burden eigenvalues
1163	**SpMin8_Bh(m)**	smallest eigenvalue n. 8 of Burden matrix weighted by mass	Burden eigenvalues
1164	**SpMin1_Bh(v)**	smallest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1165	**SpMin2_Bh(v)**	smallest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1166	**SpMin3_Bh(v)**	smallest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1167	**SpMin4_Bh(v)**	smallest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1168	**SpMin5_Bh(v)**	smallest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1169	**SpMin6_Bh(v)**	smallest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1170	**SpMin7_Bh(v)**	smallest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume	Burden eigenvalues

No.	Name	Description	Block
1171	**SpMin8_Bh(v)**	smallest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume	Burden eigenvalues
1172	**SpMin1_Bh(e)**	smallest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1173	**SpMin2_Bh(e)**	smallest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1174	**SpMin3_Bh(e)**	smallest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1175	**SpMin4_Bh(e)**	smallest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1176	**SpMin5_Bh(e)**	smallest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1177	**SpMin6_Bh(e)**	smallest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1178	**SpMin7_Bh(e)**	smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1179	**SpMin8_Bh(e)**	smallest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues
1180	**SpMin1_Bh(p)**	smallest eigenvalue n. 1 of Burden matrix weighted by polarizability	Burden eigenvalues
1181	**SpMin2_Bh(p)**	smallest eigenvalue n. 2 of Burden matrix weighted by polarizability	Burden eigenvalues
1182	**SpMin3_Bh(p)**	smallest eigenvalue n. 3 of Burden matrix weighted by polarizability	Burden eigenvalues
1183	**SpMin4_Bh(p)**	smallest eigenvalue n. 4 of Burden matrix weighted by polarizability	Burden eigenvalues
1184	**SpMin5_Bh(p)**	smallest eigenvalue n. 5 of Burden matrix weighted by polarizability	Burden eigenvalues
1185	**SpMin6_Bh(p)**	smallest eigenvalue n. 6 of Burden matrix weighted by polarizability	Burden eigenvalues
1186	**SpMin7_Bh(p)**	smallest eigenvalue n. 7 of Burden matrix weighted by polarizability	Burden eigenvalues
1187	**SpMin8_Bh(p)**	smallest eigenvalue n. 8 of Burden matrix weighted by polarizability	Burden eigenvalues
1188	**SpMin1_Bh(i)**	smallest eigenvalue n. 1 of Burden matrix weighted by ionization potential	Burden eigenvalues
1189	**SpMin2_Bh(i)**	smallest eigenvalue n. 2 of Burden matrix weighted by ionization potential	Burden eigenvalues

No.	Name	Description	Block
1190	**SpMin3_Bh(i)**	smallest eigenvalue n. 3 of Burden matrix weighted by ionization potential	Burden eigenvalues
1191	**SpMin4_Bh(i)**	smallest eigenvalue n. 4 of Burden matrix weighted by ionization potential	Burden eigenvalues
1192	**SpMin5_Bh(i)**	smallest eigenvalue n. 5 of Burden matrix weighted by ionization potential	Burden eigenvalues
1193	**SpMin6_Bh(i)**	smallest eigenvalue n. 6 of Burden matrix weighted by ionization potential	Burden eigenvalues
1194	**SpMin7_Bh(i)**	smallest eigenvalue n. 7 of Burden matrix weighted by ionization potential	Burden eigenvalues
1195	**SpMin8_Bh(i)**	smallest eigenvalue n. 8 of Burden matrix weighted by ionization potential	Burden eigenvalues
1196	**SpMin1_Bh(s)**	smallest eigenvalue n. 1 of Burden matrix weighted by I-state	Burden eigenvalues
1197	**SpMin2_Bh(s)**	smallest eigenvalue n. 2 of Burden matrix weighted by I-state	Burden eigenvalues
1198	**SpMin3_Bh(s)**	smallest eigenvalue n. 3 of Burden matrix weighted by I-state	Burden eigenvalues
1199	**SpMin4_Bh(s)**	smallest eigenvalue n. 4 of Burden matrix weighted by I-state	Burden eigenvalues
1200	**SpMin5_Bh(s)**	smallest eigenvalue n. 5 of Burden matrix weighted by I-state	Burden eigenvalues
1201	**SpMin6_Bh(s)**	smallest eigenvalue n. 6 of Burden matrix weighted by I-state	Burden eigenvalues
1202	**SpMin7_Bh(s)**	smallest eigenvalue n. 7 of Burden matrix weighted by I-state	Burden eigenvalues
1203	**SpMin8_Bh(s)**	smallest eigenvalue n. 8 of Burden matrix weighted by I-state	Burden eigenvalues
1204	**P_VSA_LogP_1**	P_VSA-like on LogP, bin 1	P_VSA-like descriptor
1205	**P_VSA_LogP_2**	P_VSA-like on LogP, bin 2	P_VSA-like descriptor
1206	**P_VSA_LogP_3**	P_VSA-like on LogP, bin 3	P_VSA-like descriptor
1207	**P_VSA_LogP_4**	P_VSA-like on LogP, bin 4	P_VSA-like descriptor
1208	**P_VSA_LogP_5**	P_VSA-like on LogP, bin 5	P_VSA-like descriptor

No.	Name	Description	Block
1209	**P_VSA_LogP_6**	P_VSA-like on LogP, bin 6	P_VSA-like descriptor
1210	**P_VSA_LogP_7**	P_VSA-like on LogP, bin 7	P_VSA-like descriptor
1211	**P_VSA_LogP_8**	P_VSA-like on LogP, bin 8	P_VSA-like descriptor
1212	**P_VSA_MR_1**	P_VSA-like on Molar Refractivity, bin 1	P_VSA-like descriptor
1213	**P_VSA_MR_2**	P_VSA-like on Molar Refractivity, bin 2	P_VSA-like descriptor
1214	**P_VSA_MR_3**	P_VSA-like on Molar Refractivity, bin 3	P_VSA-like descriptor
1215	**P_VSA_MR_4**	P_VSA-like on Molar Refractivity, bin 4	P_VSA-like descriptor
1216	**P_VSA_MR_5**	P_VSA-like on Molar Refractivity, bin 5	P_VSA-like descriptor
1217	**P_VSA_MR_6**	P_VSA-like on Molar Refractivity, bin 6	P_VSA-like descriptor
1218	**P_VSA_MR_7**	P_VSA-like on Molar Refractivity, bin 7	P_VSA-like descriptor
1219	**P_VSA_MR_8**	P_VSA-like on Molar Refractivity, bin 8	P_VSA-like descriptor
1220	**P_VSA_m_1**	P_VSA-like on mass, bin 1	P_VSA-like descriptor
1221	**P_VSA_m_2**	P_VSA-like on mass, bin 2	P_VSA-like descriptor
1222	**P_VSA_m_3**	P_VSA-like on mass, bin 3	P_VSA-like descriptor
1223	**P_VSA_m_4**	P_VSA-like on mass, bin 4	P_VSA-like descriptor
1224	**P_VSA_m_5**	P_VSA-like on mass, bin 5	P_VSA-like descriptor
1225	**P_VSA_v_1**	P_VSA-like on van der Waals volume, bin 1	P_VSA-like descriptor
1226	**P_VSA_v_2**	P_VSA-like on van der Waals volume, bin 2	P_VSA-like descriptor
1227	**P_VSA_v_3**	P_VSA-like on van der Waals volume, bin 3	P_VSA-like descriptor

No.	Name	Description	Block
1228	**P_VSA_v_4**	P_VSA-like on van der Waals volume, bin 4	P_VSA-like descriptor
1229	**P_VSA_e_1**	P_VSA-like on Sanderson electronegativity, bin 1	P_VSA-like descriptor
1230	**P_VSA_e_2**	P_VSA-like on Sanderson electronegativity, bin 2	P_VSA-like descriptor
1231	**P_VSA_e_3**	P_VSA-like on Sanderson electronegativity, bin 3	P_VSA-like descriptor
1232	**P_VSA_e_4**	P_VSA-like on Sanderson electronegativity, bin 4	P_VSA-like descriptor
1233	**P_VSA_e_5**	P_VSA-like on Sanderson electronegativity, bin 5	P_VSA-like descriptor
1234	**P_VSA_e_6**	P_VSA-like on Sanderson electronegativity, bin 6	P_VSA-like descriptor
1235	**P_VSA_p_1**	P_VSA-like on polarizability, bin 1	P_VSA-like descriptor
1236	**P_VSA_p_2**	P_VSA-like on polarizability, bin 2	P_VSA-like descriptor
1237	**P_VSA_p_3**	P_VSA-like on polarizability, bin 3	P_VSA-like descriptor
1238	**P_VSA_p_4**	P_VSA-like on polarizability, bin 4	P_VSA-like descriptor
1239	**P_VSA_i_1**	P_VSA-like on ionization potential, bin 1	P_VSA-like descriptor
1240	**P_VSA_i_2**	P_VSA-like on ionization potential, bin 2	P_VSA-like descriptor
1241	**P_VSA_i_3**	P_VSA-like on ionization potential, bin 3	P_VSA-like descriptor
1242	**P_VSA_i_4**	P_VSA-like on ionization potential, bin 4	P_VSA-like descriptor
1243	**P_VSA_s_1**	P_VSA-like on I-state, bin 1	P_VSA-like descriptor
1244	**P_VSA_s_2**	P_VSA-like on I-state, bin 2	P_VSA-like descriptor
1245	**P_VSA_s_3**	P_VSA-like on I-state, bin 3	P_VSA-like descriptor
1246	**P_VSA_s_4**	P_VSA-like on I-state, bin 4	P_VSA-like descriptor

No.	Name	Description	Block
1247	**P_VSA_s_5**	P_VSA-like on I-state, bin 5	P_VSA-like descriptor
1248	**P_VSA_s_6**	P_VSA-like on I-state, bin 6	P_VSA-like descriptor
1249	**P_VSA_ppp_L**	P_VSA-like on potential pharmacophore points, L - lipophilic	P_VSA-like descriptor
1250	**P_VSA_ppp_P**	P_VSA-like on potential pharmacophore points, P - positive	P_VSA-like descriptor
1251	**P_VSA_ppp_N**	P_VSA-like on potential pharmacophore points, N - negative	P_VSA-like descriptor
1252	**P_VSA_ppp_D**	P_VSA-like on potential pharmacophore points, D - hydrogen-bond donor	P_VSA-like descriptor
1253	**P_VSA_ppp_A**	P_VSA-like on potential pharmacophore points, A - hydrogen-bond acceptor	P_VSA-like descriptor
1254	**P_VSA_ppp_ar**	P_VSA-like on potential pharmacophore points, ar - aromatic atoms	P_VSA-like descriptor
1255	**P_VSA_ppp_con**	P_VSA-like on potential pharmacophore points, con - conjugated atoms	P_VSA-like descriptor
1256	**P_VSA_ppp_hal**	P_VSA-like on potential pharmacophore points, hal - halogen atoms	P_VSA-like descriptor
1257	**P_VSA_ppp_cyc**	P_VSA-like on potential pharmacophore points, cyc - atoms belonging to cycles	P_VSA-like descriptor
1258	**P_VSA_ppp_ter**	P_VSA-like on potential pharmacophore points, ter - terminal atoms	P_VSA-like descriptor
1259	**Eta_alpha**	eta core count	ETA indices
1260	**Eta_alpha_A**	eta average core count	ETA indices
1261	**Eta_epsi**	eta electronegativity measure	ETA indices
1262	**Eta_epsi_A**	eta average electronegativity measure	ETA indices
1263	**Eta_betaS**	eta sigma VEM count	ETA indices
1264	**Eta_betaS_A**	eta sigma average VEM coun	ETA indices
1265	**Eta_betaP**	eta pi and lone pair VEM count	ETA indices
1266	**Eta_betaP_A**	eta pi and lone pair average VEM count	ETA indices
1267	**Eta_beta**	eta VEM count	ETA indices
1268	**Eta_beta_A**	eta average VEM count	ETA indices
1269	**Eta_C**	eta composite index	ETA indices
1270	**Eta_C_A**	eta average composite index	ETA indices
1271	**Eta_L**	eta local composite index	ETA indices

No.	Name	Description	Block
1272	**Eta_L_A**	eta average local composite index	ETA indices
1273	**Eta_F**	eta functionality index	ETA indices
1274	**Eta_F_A**	eta average functionality index	ETA indices
1275	**Eta_FL**	eta local functionality index	ETA indices
1276	**Eta_FL_A**	eta average local functionality index	ETA indices
1277	**Eta_B**	eta branching index	ETA indices
1278	**Eta_B_A**	eta average branching index	ETA indices
1279	**Eta_sh_p**	eta p shape index	ETA indices
1280	**Eta_sh_y**	eta y shape index	ETA indices
1281	**Eta_sh_x**	eta x shape index	ETA indices
1282	**SpMax_EA**	leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1283	**SpMaxA_EA**	normalized leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1284	**SpDiam_EA**	spectral diameter from edge adjacency mat.	Edge adjacency indices
1285	**SpAD_EA**	spectral absolute deviation from edge adjacency mat.	Edge adjacency indices
1286	**SpMAD_EA**	spectral mean absolute deviation from edge adjacency mat.	Edge adjacency indices
1287	**SpMax_EA(ed)**	leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1288	**SpMaxA_EA(ed)**	normalized leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1289	**SpDiam_EA(ed)**	spectral diameter from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1290	**SpAD_EA(ed)**	spectral absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1291	**SpMAD_EA(ed)**	spectral mean absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1292	**SpMax_EA(bo)**	leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices
1293	**SpMaxA_EA(bo)**	normalized leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices
1294	**SpDiam_EA(bo)**	spectral diameter from edge adjacency mat. weighted by bond order	Edge adjacency indices

No.	Name	Description	Block
1295	**SpAD_EA(bo)**	spectral absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices
1296	**SpMAD_EA(bo)**	spectral mean absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices
1297	**SpMax_EA(dm)**	leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1298	**SpMaxA_EA(dm)**	normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1299	**SpDiam_EA(dm)**	spectral diameter from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1300	**SpAD_EA(dm)**	spectral absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1301	**SpMAD_EA(dm)**	spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1302	**SpMax_EA(ri)**	leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1303	**SpMaxA_EA(ri)**	normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1304	**SpDiam_EA(ri)**	spectral diameter from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1305	**SpAD_EA(ri)**	spectral absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1306	**SpMAD_EA(ri)**	spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1307	**SpMax_AEA(ed)**	leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1308	**SpMaxA_AEA(ed)**	normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1309	**SpDiam_AEA(ed)**	spectral diameter from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1310	**SpAD_AEA(ed)**	spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1311	**SpMAD_AEA(ed)**	spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1312	**SpMax_AEA(bo)**	leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1313	**SpMaxA_AEA(bo)**	normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices

No.	Name	Description	Block
1314	**SpDiam_AEA(bo)**	spectral diameter from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1315	**SpAD_AEA(bo)**	spectral absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1316	**SpMAD_AEA(bo)**	spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1317	**SpMax_AEA(dm)**	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1318	**SpMaxA_AEA(dm)**	normalized leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1319	**SpDiam_AEA(dm)**	spectral diameter from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1320	**SpAD_AEA(dm)**	spectral absolute deviation from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1321	**SpMAD_AEA(dm)**	spectral mean absolute deviation from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1322	**SpMax_AEA(ri)**	leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1323	**SpMaxA_AEA(ri)**	normalized leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1324	**SpDiam_AEA(ri)**	spectral diameter from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1325	**SpAD_AEA(ri)**	spectral absolute deviation from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1326	**SpMAD_AEA(ri)**	spectral mean absolute deviation from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1327	**Chi0_EA**	connectivity-like index of order 0 from edge adjacency mat.	Edge adjacency indices
1328	**Chi1_EA**	connectivity-like index of order 1 from edge adjacency mat.	Edge adjacency indices
1329	**Chi0_EA(ed)**	connectivity-like index of order 0 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1330	**Chi1_EA(ed)**	connectivity-like index of order 1 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1331	**Chi0_EA(bo)**	connectivity-like index of order 0 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1332	**Chi1_EA(bo)**	connectivity-like index of order 1 from edge adjacency mat. weighted by bond order	Edge adjacency indices

No.	Name	Description	Block
1333	**Chi0_EA(dm)**	connectivity-like index of order 0 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1334	**Chi1_EA(dm)**	connectivity-like index of order 1 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1335	**Chi0_EA(ri)**	connectivity-like index of order 0 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1336	**Chi1_EA(ri)**	connectivity-like index of order 1 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1337	**Chi0_AEA(ed)**	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1338	**Chi1_AEA(ed)**	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1339	**Chi0_AEA(bo)**	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1340	**Chi1_AEA(bo)**	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1341	**Chi0_AEA(dm)**	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1342	**Chi1_AEA(dm)**	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1343	**Chi0_AEA(ri)**	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1344	**Chi1_AEA(ri)**	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1345	**SM02_EA**	spectral moment of order 2 from edge adjacency mat.	Edge adjacency indices
1346	**SM03_EA**	spectral moment of order 3 from edge adjacency mat.	Edge adjacency indices
1347	**SM04_EA**	spectral moment of order 4 from edge adjacency mat.	Edge adjacency indices
1348	**SM05_EA**	spectral moment of order 5 from edge adjacency mat.	Edge adjacency indices
1349	**SM06_EA**	spectral moment of order 6 from edge adjacency mat.	Edge adjacency indices
1350	**SM07_EA**	spectral moment of order 7 from edge adjacency mat.	Edge adjacency indices
1351	**SM08_EA**	spectral moment of order 8 from edge adjacency mat.	Edge adjacency indices

No.	Name	Description	Block
1352	**SM09_EA**	spectral moment of order 9 from edge adjacency mat.	Edge adjacency indices
1353	**SM10_EA**	spectral moment of order 10 from edge adjacency mat.	Edge adjacency indices
1354	**SM11_EA**	spectral moment of order 11 from edge adjacency mat.	Edge adjacency indices
1355	**SM12_EA**	spectral moment of order 12 from edge adjacency mat.	Edge adjacency indices
1356	**SM13_EA**	spectral moment of order 13 from edge adjacency mat.	Edge adjacency indices
1357	**SM14_EA**	spectral moment of order 14 from edge adjacency mat.	Edge adjacency indices
1358	**SM15_EA**	spectral moment of order 15 from edge adjacency mat.	Edge adjacency indices
1359	**SM02_EA(ed)**	spectral moment of order 2 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1360	**SM03_EA(ed)**	spectral moment of order 3 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1361	**SM04_EA(ed)**	spectral moment of order 4 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1362	**SM05_EA(ed)**	spectral moment of order 5 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1363	**SM06_EA(ed)**	spectral moment of order 6 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1364	**SM07_EA(ed)**	spectral moment of order 7 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1365	**SM08_EA(ed)**	spectral moment of order 8 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1366	**SM09_EA(ed)**	spectral moment of order 9 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1367	**SM10_EA(ed)**	spectral moment of order 10 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1368	**SM11_EA(ed)**	spectral moment of order 11 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1369	**SM12_EA(ed)**	spectral moment of order 12 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1370	**SM13_EA(ed)**	spectral moment of order 13 from edge adjacency mat. weighted by edge degree	Edge adjacency indices

No.	Name	Description	Block
1371	**SM14_EA(ed)**	spectral moment of order 14 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1372	**SM15_EA(ed)**	spectral moment of order 15 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1373	**SM02_EA(bo)**	spectral moment of order 2 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1374	**SM03_EA(bo)**	spectral moment of order 3 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1375	**SM04_EA(bo)**	spectral moment of order 4 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1376	**SM05_EA(bo)**	spectral moment of order 5 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1377	**SM06_EA(bo)**	spectral moment of order 6 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1378	**SM07_EA(bo)**	spectral moment of order 7 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1379	**SM08_EA(bo)**	spectral moment of order 8 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1380	**SM09_EA(bo)**	spectral moment of order 9 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1381	**SM10_EA(bo)**	spectral moment of order 10 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1382	**SM11_EA(bo)**	spectral moment of order 11 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1383	**SM12_EA(bo)**	spectral moment of order 12 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1384	**SM13_EA(bo)**	spectral moment of order 13 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1385	**SM14_EA(bo)**	spectral moment of order 14 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1386	**SM15_EA(bo)**	spectral moment of order 15 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1387	**SM02_EA(dm)**	spectral moment of order 2 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1388	**SM03_EA(dm)**	spectral moment of order 3 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1389	**SM04_EA(dm)**	spectral moment of order 4 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices

No.	Name	Description	Block
1390	**SM05_EA(dm)**	spectral moment of order 5 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1391	**SM06_EA(dm)**	spectral moment of order 6 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1392	**SM07_EA(dm)**	spectral moment of order 7 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1393	**SM08_EA(dm)**	spectral moment of order 8 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1394	**SM09_EA(dm)**	spectral moment of order 9 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1395	**SM10_EA(dm)**	spectral moment of order 10 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1396	**SM11_EA(dm)**	spectral moment of order 11 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1397	**SM12_EA(dm)**	spectral moment of order 12 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1398	**SM13_EA(dm)**	spectral moment of order 13 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1399	**SM14_EA(dm)**	spectral moment of order 14 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1400	**SM15_EA(dm)**	spectral moment of order 15 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1401	**SM02_EA(ri)**	spectral moment of order 2 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1402	**SM03_EA(ri)**	spectral moment of order 3 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1403	**SM04_EA(ri)**	spectral moment of order 4 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1404	**SM05_EA(ri)**	spectral moment of order 5 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1405	**SM06_EA(ri)**	spectral moment of order 6 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1406	**SM07_EA(ri)**	spectral moment of order 7 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1407	**SM08_EA(ri)**	spectral moment of order 8 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1408	**SM09_EA(ri)**	spectral moment of order 9 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices

No.	Name	Description	Block
1409	**SM10_EA(ri)**	spectral moment of order 10 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1410	**SM11_EA(ri)**	spectral moment of order 11 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1411	**SM12_EA(ri)**	spectral moment of order 12 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1412	**SM13_EA(ri)**	spectral moment of order 13 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1413	**SM14_EA(ri)**	spectral moment of order 14 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1414	**SM15_EA(ri)**	spectral moment of order 15 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1415	**SM02_AEA(ed)**	spectral moment of order 2 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1416	**SM03_AEA(ed)**	spectral moment of order 3 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1417	**SM04_AEA(ed)**	spectral moment of order 4 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1418	**SM05_AEA(ed)**	spectral moment of order 5 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1419	**SM06_AEA(ed)**	spectral moment of order 6 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1420	**SM07_AEA(ed)**	spectral moment of order 7 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1421	**SM08_AEA(ed)**	spectral moment of order 8 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1422	**SM09_AEA(ed)**	spectral moment of order 9 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1423	**SM10_AEA(ed)**	spectral moment of order 10 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1424	**SM11_AEA(ed)**	spectral moment of order 11 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1425	**SM12_AEA(ed)**	spectral moment of order 12 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1426	**SM13_AEA(ed)**	spectral moment of order 13 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1427	**SM14_AEA(ed)**	spectral moment of order 14 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices

No.	Name	Description	Block
1428	**SM15_AEA(ed)**	spectral moment of order 15 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1429	**SM02_AEA(bo)**	spectral moment of order 2 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1430	**SM03_AEA(bo)**	spectral moment of order 3 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1431	**SM04_AEA(bo)**	spectral moment of order 4 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1432	**SM05_AEA(bo)**	spectral moment of order 5 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1433	**SM06_AEA(bo)**	spectral moment of order 6 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1434	**SM07_AEA(bo)**	spectral moment of order 7 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1435	**SM08_AEA(bo)**	spectral moment of order 8 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1436	**SM09_AEA(bo)**	spectral moment of order 9 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1437	**SM10_AEA(bo)**	spectral moment of order 10 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1438	**SM11_AEA(bo)**	spectral moment of order 11 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1439	**SM12_AEA(bo)**	spectral moment of order 12 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1440	**SM13_AEA(bo)**	spectral moment of order 13 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1441	**SM14_AEA(bo)**	spectral moment of order 14 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1442	**SM15_AEA(bo)**	spectral moment of order 15 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1443	**SM02_AEA(dm)**	spectral moment of order 2 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1444	**SM03_AEA(dm)**	spectral moment of order 3 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1445	**SM04_AEA(dm)**	spectral moment of order 4 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1446	**SM05_AEA(dm)**	spectral moment of order 5 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices

No.	Name	Description	Block
1447	**SM06_AEA(dm)**	spectral moment of order 6 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1448	**SM07_AEA(dm)**	spectral moment of order 7 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1449	**SM08_AEA(dm)**	spectral moment of order 8 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1450	**SM09_AEA(dm)**	spectral moment of order 9 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1451	**SM10_AEA(dm)**	spectral moment of order 10 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1452	**SM11_AEA(dm)**	spectral moment of order 11 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1453	**SM12_AEA(dm)**	spectral moment of order 12 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1454	**SM13_AEA(dm)**	spectral moment of order 13 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1455	**SM14_AEA(dm)**	spectral moment of order 14 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1456	**SM15_AEA(dm)**	spectral moment of order 15 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1457	**SM02_AEA(ri)**	spectral moment of order 2 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1458	**SM03_AEA(ri)**	spectral moment of order 3 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1459	**SM04_AEA(ri)**	spectral moment of order 4 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1460	**SM05_AEA(ri)**	spectral moment of order 5 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1461	**SM06_AEA(ri)**	spectral moment of order 6 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1462	**SM07_AEA(ri)**	spectral moment of order 7 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1463	**SM08_AEA(ri)**	spectral moment of order 8 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1464	**SM09_AEA(ri)**	spectral moment of order 9 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1465	**SM10_AEA(ri)**	spectral moment of order 10 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices

No.	Name	Description	Block
1466	**SM11_AEA(ri)**	spectral moment of order 11 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1467	**SM12_AEA(ri)**	spectral moment of order 12 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1468	**SM13_AEA(ri)**	spectral moment of order 13 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1469	**SM14_AEA(ri)**	spectral moment of order 14 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1470	**SM15_AEA(ri)**	spectral moment of order 15 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1471	**Eig01_EA**	eigenvalue n. 1 from edge adjacency mat.	Edge adjacency indices
1472	**Eig02_EA**	eigenvalue n. 2 from edge adjacency mat.	Edge adjacency indices
1473	**Eig03_EA**	eigenvalue n. 3 from edge adjacency mat.	Edge adjacency indices
1474	**Eig04_EA**	eigenvalue n. 4 from edge adjacency mat.	Edge adjacency indices
1475	**Eig05_EA**	eigenvalue n. 5 from edge adjacency mat.	Edge adjacency indices
1476	**Eig06_EA**	eigenvalue n. 6 from edge adjacency mat.	Edge adjacency indices
1477	**Eig07_EA**	eigenvalue n. 7 from edge adjacency mat.	Edge adjacency indices
1478	**Eig08_EA**	eigenvalue n. 8 from edge adjacency mat.	Edge adjacency indices
1479	**Eig09_EA**	eigenvalue n. 9 from edge adjacency mat.	Edge adjacency indices
1480	**Eig10_EA**	eigenvalue n. 10 from edge adjacency mat.	Edge adjacency indices
1481	**Eig11_EA**	eigenvalue n. 11 from edge adjacency mat.	Edge adjacency indices
1482	**Eig12_EA**	eigenvalue n. 12 from edge adjacency mat.	Edge adjacency indices
1483	**Eig13_EA**	eigenvalue n. 13 from edge adjacency mat.	Edge adjacency indices
1484	**Eig14_EA**	eigenvalue n. 14 from edge adjacency mat.	Edge adjacency indices

No.	Name	Description	Block
1485	**Eig15_EA**	eigenvalue n. 15 from edge adjacency mat.	Edge adjacency indices
1486	**Eig01_EA(ed)**	eigenvalue n. 1 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1487	**Eig02_EA(ed)**	eigenvalue n. 2 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1488	**Eig03_EA(ed)**	eigenvalue n. 3 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1489	**Eig04_EA(ed)**	eigenvalue n. 4 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1490	**Eig05_EA(ed)**	eigenvalue n. 5 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1491	**Eig06_EA(ed)**	eigenvalue n. 6 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1492	**Eig07_EA(ed)**	eigenvalue n. 7 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1493	**Eig08_EA(ed)**	eigenvalue n. 8 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1494	**Eig09_EA(ed)**	eigenvalue n. 9 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1495	**Eig10_EA(ed)**	eigenvalue n. 10 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1496	**Eig11_EA(ed)**	eigenvalue n. 11 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1497	**Eig12_EA(ed)**	eigenvalue n. 12 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1498	**Eig13_EA(ed)**	eigenvalue n. 13 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1499	**Eig14_EA(ed)**	eigenvalue n. 14 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1500	**Eig15_EA(ed)**	eigenvalue n. 15 from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1501	**Eig01_EA(bo)**	eigenvalue n. 1 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1502	**Eig02_EA(bo)**	eigenvalue n. 2 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1503	**Eig03_EA(bo)**	eigenvalue n. 3 from edge adjacency mat. weighted by bond order	Edge adjacency indices

No.	Name	Description	Block
1504	**Eig04_EA(bo)**	eigenvalue n. 4 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1505	**Eig05_EA(bo)**	eigenvalue n. 5 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1506	**Eig06_EA(bo)**	eigenvalue n. 6 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1507	**Eig07_EA(bo)**	eigenvalue n. 7 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1508	**Eig08_EA(bo)**	eigenvalue n. 8 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1509	**Eig09_EA(bo)**	eigenvalue n. 9 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1510	**Eig10_EA(bo)**	eigenvalue n. 10 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1511	**Eig11_EA(bo)**	eigenvalue n. 11 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1512	**Eig12_EA(bo)**	eigenvalue n. 12 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1513	**Eig13_EA(bo)**	eigenvalue n. 13 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1514	**Eig14_EA(bo)**	eigenvalue n. 14 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1515	**Eig15_EA(bo)**	eigenvalue n. 15 from edge adjacency mat. weighted by bond order	Edge adjacency indices
1516	**Eig01_EA(dm)**	eigenvalue n. 1 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1517	**Eig02_EA(dm)**	eigenvalue n. 2 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1518	**Eig03_EA(dm)**	eigenvalue n. 3 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1519	**Eig04_EA(dm)**	eigenvalue n. 4 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1520	**Eig05_EA(dm)**	eigenvalue n. 5 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1521	**Eig06_EA(dm)**	eigenvalue n. 6 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1522	**Eig07_EA(dm)**	eigenvalue n. 7 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices

No.	Name	Description	Block
1523	**Eig08_EA(dm)**	eigenvalue n. 8 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1524	**Eig09_EA(dm)**	eigenvalue n. 9 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1525	**Eig10_EA(dm)**	eigenvalue n. 10 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1526	**Eig11_EA(dm)**	eigenvalue n. 11 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1527	**Eig12_EA(dm)**	eigenvalue n. 12 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1528	**Eig13_EA(dm)**	eigenvalue n. 13 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1529	**Eig14_EA(dm)**	eigenvalue n. 14 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1530	**Eig15_EA(dm)**	eigenvalue n. 15 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1531	**Eig01_EA(ri)**	eigenvalue n. 1 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1532	**Eig02_EA(ri)**	eigenvalue n. 2 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1533	**Eig03_EA(ri)**	eigenvalue n. 3 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1534	**Eig04_EA(ri)**	eigenvalue n. 4 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1535	**Eig05_EA(ri)**	eigenvalue n. 5 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1536	**Eig06_EA(ri)**	eigenvalue n. 6 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1537	**Eig07_EA(ri)**	eigenvalue n. 7 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1538	**Eig08_EA(ri)**	eigenvalue n. 8 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1539	**Eig09_EA(ri)**	eigenvalue n. 9 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1540	**Eig10_EA(ri)**	eigenvalue n. 10 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1541	**Eig11_EA(ri)**	eigenvalue n. 11 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices

No.	Name	Description	Block
1542	**Eig12_EA(ri)**	eigenvalue n. 12 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1543	**Eig13_EA(ri)**	eigenvalue n. 13 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1544	**Eig14_EA(ri)**	eigenvalue n. 14 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1545	**Eig15_EA(ri)**	eigenvalue n. 15 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1546	**Eig01_AEA(ed)**	eigenvalue n. 1 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1547	**Eig02_AEA(ed)**	eigenvalue n. 2 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1548	**Eig03_AEA(ed)**	eigenvalue n. 3 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1549	**Eig04_AEA(ed)**	eigenvalue n. 4 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1550	**Eig05_AEA(ed)**	eigenvalue n. 5 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1551	**Eig06_AEA(ed)**	eigenvalue n. 6 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1552	**Eig07_AEA(ed)**	eigenvalue n. 7 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1553	**Eig08_AEA(ed)**	eigenvalue n. 8 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1554	**Eig09_AEA(ed)**	eigenvalue n. 9 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1555	**Eig10_AEA(ed)**	eigenvalue n. 10 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1556	**Eig11_AEA(ed)**	eigenvalue n. 11 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1557	**Eig12_AEA(ed)**	eigenvalue n. 12 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1558	**Eig13_AEA(ed)**	eigenvalue n. 13 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1559	**Eig14_AEA(ed)**	eigenvalue n. 14 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1560	**Eig15_AEA(ed)**	eigenvalue n. 15 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices

No.	Name	Description	Block
1561	**Eig01_AEA(bo)**	eigenvalue n. 1 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1562	**Eig02_AEA(bo)**	eigenvalue n. 2 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1563	**Eig03_AEA(bo)**	eigenvalue n. 3 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1564	**Eig04_AEA(bo)**	eigenvalue n. 4 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1565	**Eig05_AEA(bo)**	eigenvalue n. 5 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1566	**Eig06_AEA(bo)**	eigenvalue n. 6 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1567	**Eig07_AEA(bo)**	eigenvalue n. 7 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1568	**Eig08_AEA(bo)**	eigenvalue n. 8 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1569	**Eig09_AEA(bo)**	eigenvalue n. 9 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1570	**Eig10_AEA(bo)**	eigenvalue n. 10 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1571	**Eig11_AEA(bo)**	eigenvalue n. 11 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1572	**Eig12_AEA(bo)**	eigenvalue n. 12 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1573	**Eig13_AEA(bo)**	eigenvalue n. 13 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1574	**Eig14_AEA(bo)**	eigenvalue n. 14 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1575	**Eig15_AEA(bo)**	eigenvalue n. 15 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1576	**Eig01_AEA(dm)**	eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1577	**Eig02_AEA(dm)**	eigenvalue n. 2 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1578	**Eig03_AEA(dm)**	eigenvalue n. 3 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1579	**Eig04_AEA(dm)**	eigenvalue n. 4 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices

No.	Name	Description	Block
1580	**Eig05_AEA(dm)**	eigenvalue n. 5 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1581	**Eig06_AEA(dm)**	eigenvalue n. 6 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1582	**Eig07_AEA(dm)**	eigenvalue n. 7 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1583	**Eig08_AEA(dm)**	eigenvalue n. 8 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1584	**Eig09_AEA(dm)**	eigenvalue n. 9 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1585	**Eig10_AEA(dm)**	eigenvalue n. 10 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1586	**Eig11_AEA(dm)**	eigenvalue n. 11 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1587	**Eig12_AEA(dm)**	eigenvalue n. 12 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1588	**Eig13_AEA(dm)**	eigenvalue n. 13 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1589	**Eig14_AEA(dm)**	eigenvalue n. 14 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1590	**Eig15_AEA(dm)**	eigenvalue n. 15 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1591	**Eig01_AEA(ri)**	eigenvalue n. 1 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1592	**Eig02_AEA(ri)**	eigenvalue n. 2 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1593	**Eig03_AEA(ri)**	eigenvalue n. 3 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1594	**Eig04_AEA(ri)**	eigenvalue n. 4 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1595	**Eig05_AEA(ri)**	eigenvalue n. 5 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1596	**Eig06_AEA(ri)**	eigenvalue n. 6 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1597	**Eig07_AEA(ri)**	eigenvalue n. 7 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1598	**Eig08_AEA(ri)**	eigenvalue n. 8 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices

No.	Name	Description	Block
1599	**Eig09_AEA(ri)**	eigenvalue n. 9 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1600	**Eig10_AEA(ri)**	eigenvalue n. 10 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1601	**Eig11_AEA(ri)**	eigenvalue n. 11 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1602	**Eig12_AEA(ri)**	eigenvalue n. 12 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1603	**Eig13_AEA(ri)**	eigenvalue n. 13 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1604	**Eig14_AEA(ri)**	eigenvalue n. 14 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1605	**Eig15_AEA(ri)**	eigenvalue n. 15 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1606	**G1**	gravitational index G1	Geometrical descriptors
1607	**G2**	gravitational index G2 (bond-restricted)	Geometrical descriptors
1608	**RGyr**	radius of gyration (mass weighted)	Geometrical descriptors
1609	**SPAN**	span R	Geometrical descriptors
1610	**SPAM**	average span R	Geometrical descriptors
1611	**MEcc**	molecular eccentricity	Geometrical descriptors
1612	**SPH**	spherosity	Geometrical descriptors
1613	**ASP**	asphericity	Geometrical descriptors
1614	**PJI3**	3D Petitjean shape index	Geometrical descriptors
1615	**L/Bw**	length-to-breadth ratio by WHIM	Geometrical descriptors
1616	**HOMA**	Harmonic Oscillator Model of Aromaticity index	Geometrical descriptors
1617	**CMBL**	conjugated maximum bond length	Geometrical descriptors

No.	Name	Description	Block
1618	**AROM**	aromaticity index	Geometrical descriptors
1619	**HOMT**	HOMA total	Geometrical descriptors
1620	**DISPm**	displacement value / weighted by mass	Geometrical descriptors
1621	**QXXm**	quadrupole x-component value / weighted by mass	Geometrical descriptors
1622	**QYYm**	quadrupole y-component value / weighted by mass	Geometrical descriptors
1623	**QZZm**	quadrupole z-component value / weighted by mass	Geometrical descriptors
1624	**DISPv**	displacement value / weighted by van der Waals volume	Geometrical descriptors
1625	**QXXv**	quadrupole x-component value / weighted by van der Waals volume	Geometrical descriptors
1626	**QYYv**	quadrupole y-component value / weighted by van der Waals volume	Geometrical descriptors
1627	**QZZv**	quadrupole z-component value / weighted by van der Waals volume	Geometrical descriptors
1628	**DISPe**	displacement value / weighted by Sanderson electronegativity	Geometrical descriptors
1629	**QXXe**	quadrupole x-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1630	**QYYe**	quadrupole y-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1631	**QZZe**	quadrupole z-component value / weighted by Sanderson electronegativity	Geometrical descriptors
1632	**DISPp**	displacement value / weighted by polarizability	Geometrical descriptors
1633	**QXXp**	quadrupole x-component value / weighted by polarizability	Geometrical descriptors
1634	**QYYp**	quadrupole y-component value / weighted by polarizability	Geometrical descriptors
1635	**QZZp**	quadrupole z-component value / weighted by polarizability	Geometrical descriptors
1636	**DISPi**	displacement value / weighted by ionization potential	Geometrical descriptors

No.	Name	Description	Block
1637	**QXXi**	quadrupole x-component value / weighted by ionization potential	Geometrical descriptors
1638	**QYYi**	quadrupole y-component value / weighted by ionization potential	Geometrical descriptors
1639	**QZZi**	quadrupole z-component value / weighted by ionization potential	Geometrical descriptors
1640	**DISPs**	displacement value / weighted by I-state	Geometrical descriptors
1641	**QXXs**	quadrupole x-component value / weighted by I-state	Geometrical descriptors
1642	**QYYs**	quadrupole y-component value / weighted by I-state	Geometrical descriptors
1643	**QZZs**	quadrupole z-component value / weighted by I-state	Geometrical descriptors
1644	**Wi_G**	Wiener-like index from geometrical matrix	3D matrix-based descriptors
1645	**WiA_G**	average Wiener-like index from geometrical matrix	3D matrix-based descriptors
1646	**AVS_G**	average vertex sum from geometrical matrix	3D matrix-based descriptors
1647	**H_G**	Harary-like index from geometrical matrix	3D matrix-based descriptors
1648	**Chi_G**	Randic-like index from geometrical matrix	3D matrix-based descriptors
1649	**ChiA_G**	average Randic-like index from geometrical matrix	3D matrix-based descriptors
1650	**J_G**	Balaban-like index from geometrical matrix	3D matrix-based descriptors
1651	**HyWi_G**	hyper-Wiener-like index from geometrical matrix	3D matrix-based descriptors
1652	**SpAbs_G**	graph energy from geometrical matrix	3D matrix-based descriptors

No.	Name	Description	Block
1653	**SpPos_G**	spectral positive sum from geometrical matrix	3D matrix-based descriptors
1654	**SpPosA_G**	normalized spectral positive sum from geometrical matrix	3D matrix-based descriptors
1655	**SpPosLog_G**	logarithmic spectral positive sum from geometrical matrix	3D matrix-based descriptors
1656	**SpMax_G**	leading eigenvalue from geometrical matrix	3D matrix-based descriptors
1657	**SpMaxA_G**	normalized leading eigenvalue from geometrical matrix	3D matrix-based descriptors
1658	**SpDiam_G**	spectral diameter from geometrical matrix	3D matrix-based descriptors
1659	**SpAD_G**	spectral absolute deviation from geometrical matrix	3D matrix-based descriptors
1660	**SpMAD_G**	spectral mean absolute deviation from geometrical matrix	3D matrix-based descriptors
1661	**Ho_G**	Hosoya-like index (log function) from geometrical matrix	3D matrix-based descriptors
1662	**EE_G**	Estrada-like index (log function) from geometrical matrix	3D matrix-based descriptors
1663	**SM2_G**	spectral moment of order 2 from geometrical matrix	3D matrix-based descriptors
1664	**SM3_G**	spectral moment of order 3 from geometrical matrix	3D matrix-based descriptors
1665	**SM4_G**	spectral moment of order 4 from geometrical matrix	3D matrix-based descriptors
1666	**SM5_G**	spectral moment of order 5 from geometrical matrix	3D matrix-based descriptors

No.	Name	Description	Block
1667	**SM6_G**	spectral moment of order 6 from geometrical matrix	3D matrix-based descriptors
1668	**VE1_G**	coefficient sum of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors
1669	**VE2_G**	average coefficient of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors
1670	**VE3_G**	logarithmic coefficient sum of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors
1671	**VE1sign_G**	coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1672	**VE2sign_G**	average coefficient of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1673	**VE3sign_G**	logarithmic coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors
1674	**VR1_G**	Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1675	**VR2_G**	normalized Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1676	**VR3_G**	logarithmic Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors
1677	**Wi_RG**	Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1678	**WiA_RG**	average Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1679	**AVS_RG**	average vertex sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1680	**H_RG**	Harary-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors

No.	Name	Description	Block
1681	**Chi_RG**	Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1682	**ChiA_RG**	average Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1683	**J_RG**	Balaban-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1684	**HyWi_RG**	hyper-Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1685	**SpAbs_RG**	graph energy from reciprocal squared geometrical matrix	3D matrix-based descriptors
1686	**SpPos_RG**	spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1687	**SpPosA_RG**	normalized spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1688	**SpPosLog_RG**	logarithmic spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors
1689	**SpMax_RG**	leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors
1690	**SpMaxA_RG**	normalized leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors
1691	**SpDiam_RG**	spectral diameter from reciprocal squared geometrical matrix	3D matrix-based descriptors
1692	**SpAD_RG**	spectral absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors
1693	**SpMAD_RG**	spectral mean absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors
1694	**Ho_RG**	Hosoya-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors

No.	Name	Description	Block
1695	**EE_RG**	Estrada-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1696	**SM2_RG**	spectral moment of order 2 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1697	**SM3_RG**	spectral moment of order 3 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1698	**SM4_RG**	spectral moment of order 4 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1699	**SM5_RG**	spectral moment of order 5 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1700	**SM6_RG**	spectral moment of order 6 from reciprocal squared geometrical matrix	3D matrix-based descriptors
1701	**VE1_RG**	coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1702	**VE2_RG**	average coefficient of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1703	**VE3_RG**	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors
1704	**VE1sign_RG**	coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1705	**VE2sign_RG**	average coefficient of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1706	**VE3sign_RG**	logarithmic coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors
1707	**VR1_RG**	Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1708	**VR2_RG**	normalized Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors

No.	Name	Description	Block
1709	**VR3_RG**	logarithmic Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors
1710	**Wi_G/D**	Wiener-like index from distance/distance matrix	3D matrix-based descriptors
1711	**WiA_G/D**	average Wiener-like index from distance/distance matrix	3D matrix-based descriptors
1712	**AVS_G/D**	average vertex sum from distance/distance matrix	3D matrix-based descriptors
1713	**H_G/D**	Harary-like index from distance/distance matrix	3D matrix-based descriptors
1714	**Chi_G/D**	Randic-like index from distance/distance matrix	3D matrix-based descriptors
1715	**ChiA_G/D**	average Randic-like index from distance/distance matrix	3D matrix-based descriptors
1716	**J_G/D**	Balaban-like index from distance/distance matrix	3D matrix-based descriptors
1717	**HyWi_G/D**	hyper-Wiener-like index from distance/distance matrix	3D matrix-based descriptors
1718	**SpAbs_G/D**	graph energy from distance/distance matrix	3D matrix-based descriptors
1719	**SpPos_G/D**	spectral positive sum from distance/distance matrix	3D matrix-based descriptors
1720	**SpPosA_G/D**	normalized spectral positive sum from distance/distance matrix	3D matrix-based descriptors
1721	**SpPosLog_G/D**	logarithmic spectral positive sum from distance/distance matrix	3D matrix-based descriptors
1722	**SpMax_G/D**	leading eigenvalue from distance/distance matrix	3D matrix-based descriptors

No.	Name	Description	Block
1723	**SpMaxA_G/D**	normalized leading eigenvalue from distance/distance matrix (folding degree index)	3D matrix-based descriptors
1724	**SpDiam_G/D**	spectral diameter from distance/distance matrix	3D matrix-based descriptors
1725	**SpAD_G/D**	spectral absolute deviation from distance/distance matrix	3D matrix-based descriptors
1726	**SpMAD_G/D**	spectral mean absolute deviation from distance/distance matrix	3D matrix-based descriptors
1727	**Ho_G/D**	Hosoya-like index (log function) from distance/distance matrix	3D matrix-based descriptors
1728	**EE_G/D**	Estrada-like index (log function) from distance/distance matrix	3D matrix-based descriptors
1729	**SM2_G/D**	spectral moment of order 2 from distance/distance matrix	3D matrix-based descriptors
1730	**SM3_G/D**	spectral moment of order 3 from distance/distance matrix	3D matrix-based descriptors
1731	**SM4_G/D**	spectral moment of order 4 from distance/distance matrix	3D matrix-based descriptors
1732	**SM5_G/D**	spectral moment of order 5 from distance/distance matrix	3D matrix-based descriptors
1733	**SM6_G/D**	spectral moment of order 6 from distance/distance matrix	3D matrix-based descriptors
1734	**VE1_G/D**	coefficient sum of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors
1735	**VE2_G/D**	average coefficient of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors
1736	**VE3_G/D**	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors

No.	Name	Description	Block
1737	**VE1sign_G/D**	coefficient sum of the last eigenvector from distance/distance matrix	3D matrix-based descriptors
1738	**VE2sign_G/D**	average coefficient of the last eigenvector from distance/distance matrix	3D matrix-based descriptors
1739	**VE3sign_G/D**	logarithmic coefficient sum of the last eigenvector from distance/distance matrix	3D matrix-based descriptors
1740	**VR1_G/D**	Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors
1741	**VR2_G/D**	normalized Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors
1742	**VR3_G/D**	logarithmic Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors
1743	**TDB01u**	3D Topological distance based descriptors - lag 1 unweighted	3D autocorrelations
1744	**TDB02u**	3D Topological distance based descriptors - lag 2 unweighted	3D autocorrelations
1745	**TDB03u**	3D Topological distance based descriptors - lag 3 unweighted	3D autocorrelations
1746	**TDB04u**	3D Topological distance based descriptors - lag 4 unweighted	3D autocorrelations
1747	**TDB05u**	3D Topological distance based descriptors - lag 5 unweighted	3D autocorrelations
1748	**TDB06u**	3D Topological distance based descriptors - lag 6 unweighted	3D autocorrelations
1749	**TDB07u**	3D Topological distance based descriptors - lag 7 unweighted	3D autocorrelations
1750	**TDB08u**	3D Topological distance based descriptors - lag 8 unweighted	3D autocorrelations
1751	**TDB09u**	3D Topological distance based descriptors - lag 9 unweighted	3D autocorrelations
1752	**TDB10u**	3D Topological distance based descriptors - lag 10 unweighted	3D autocorrelations
1753	**TDB01m**	3D Topological distance based descriptors - lag 1 weighted by mass	3D autocorrelations

No.	Name	Description	Block
1754	**TDB02m**	3D Topological distance based descriptors - lag 2 weighted by mass	3D autocorrelations
1755	**TDB03m**	3D Topological distance based descriptors - lag 3 weighted by mass	3D autocorrelations
1756	**TDB04m**	3D Topological distance based descriptors - lag 4 weighted by mass	3D autocorrelations
1757	**TDB05m**	3D Topological distance based descriptors - lag 5 weighted by mass	3D autocorrelations
1758	**TDB06m**	3D Topological distance based descriptors - lag 6 weighted by mass	3D autocorrelations
1759	**TDB07m**	3D Topological distance based descriptors - lag 7 weighted by mass	3D autocorrelations
1760	**TDB08m**	3D Topological distance based descriptors - lag 8 weighted by mass	3D autocorrelations
1761	**TDB09m**	3D Topological distance based descriptors - lag 9 weighted by mass	3D autocorrelations
1762	**TDB10m**	3D Topological distance based descriptors - lag 10 weighted by mass	3D autocorrelations
1763	**TDB01v**	3D Topological distance based descriptors - lag 1 weighted by van der Waals volume	3D autocorrelations
1764	**TDB02v**	3D Topological distance based descriptors - lag 2 weighted by van der Waals volume	3D autocorrelations
1765	**TDB03v**	3D Topological distance based descriptors - lag 3 weighted by van der Waals volume	3D autocorrelations
1766	**TDB04v**	3D Topological distance based descriptors - lag 4 weighted by van der Waals volume	3D autocorrelations
1767	**TDB05v**	3D Topological distance based descriptors - lag 5 weighted by van der Waals volume	3D autocorrelations
1768	**TDB06v**	3D Topological distance based descriptors - lag 6 weighted by van der Waals volume	3D autocorrelations
1769	**TDB07v**	3D Topological distance based descriptors - lag 7 weighted by van der Waals volume	3D autocorrelations
1770	**TDB08v**	3D Topological distance based descriptors - lag 8 weighted by van der Waals volume	3D autocorrelations
1771	**TDB09v**	3D Topological distance based descriptors - lag 9 weighted by van der Waals volume	3D autocorrelations
1772	**TDB10v**	3D Topological distance based descriptors - lag 10 weighted by van der Waals volume	3D autocorrelations

No.	Name	Description	Block
1773	**TDB01e**	3D Topological distance based descriptors - lag 1 weighted by Sanderson electronegativity	3D autocorrelations
1774	**TDB02e**	3D Topological distance based descriptors - lag 2 weighted by Sanderson electronegativity	3D autocorrelations
1775	**TDB03e**	3D Topological distance based descriptors - lag 3 weighted by Sanderson electronegativity	3D autocorrelations
1776	**TDB04e**	3D Topological distance based descriptors - lag 4 weighted by Sanderson electronegativity	3D autocorrelations
1777	**TDB05e**	3D Topological distance based descriptors - lag 5 weighted by Sanderson electronegativity	3D autocorrelations
1778	**TDB06e**	3D Topological distance based descriptors - lag 6 weighted by Sanderson electronegativity	3D autocorrelations
1779	**TDB07e**	3D Topological distance based descriptors - lag 7 weighted by Sanderson electronegativity	3D autocorrelations
1780	**TDB08e**	3D Topological distance based descriptors - lag 8 weighted by Sanderson electronegativity	3D autocorrelations
1781	**TDB09e**	3D Topological distance based descriptors - lag 9 weighted by Sanderson electronegativity	3D autocorrelations
1782	**TDB10e**	3D Topological distance based descriptors - lag 10 weighted by Sanderson electronegativity	3D autocorrelations
1783	**TDB01p**	3D Topological distance based descriptors - lag 1 weighted by polarizability	3D autocorrelations
1784	**TDB02p**	3D Topological distance based descriptors - lag 2 weighted by polarizability	3D autocorrelations
1785	**TDB03p**	3D Topological distance based descriptors - lag 3 weighted by polarizability	3D autocorrelations
1786	**TDB04p**	3D Topological distance based descriptors - lag 4 weighted by polarizability	3D autocorrelations
1787	**TDB05p**	3D Topological distance based descriptors - lag 5 weighted by polarizability	3D autocorrelations
1788	**TDB06p**	3D Topological distance based descriptors - lag 6 weighted by polarizability	3D autocorrelations
1789	**TDB07p**	3D Topological distance based descriptors - lag 7 weighted by polarizability	3D autocorrelations
1790	**TDB08p**	3D Topological distance based descriptors - lag 8 weighted by polarizability	3D autocorrelations
1791	**TDB09p**	3D Topological distance based descriptors - lag 9 weighted by polarizability	3D autocorrelations

No.	Name	Description	Block
1792	**TDB10p**	3D Topological distance based descriptors - lag 10 weighted by polarizability	3D autocorrelations
1793	**TDB01i**	3D Topological distance based descriptors - lag 1 weighted by ionization potential	3D autocorrelations
1794	**TDB02i**	3D Topological distance based descriptors - lag 2 weighted by ionization potential	3D autocorrelations
1795	**TDB03i**	3D Topological distance based descriptors - lag 3 weighted by ionization potential	3D autocorrelations
1796	**TDB04i**	3D Topological distance based descriptors - lag 4 weighted by ionization potential	3D autocorrelations
1797	**TDB05i**	3D Topological distance based descriptors - lag 5 weighted by ionization potential	3D autocorrelations
1798	**TDB06i**	3D Topological distance based descriptors - lag 6 weighted by ionization potential	3D autocorrelations
1799	**TDB07i**	3D Topological distance based descriptors - lag 7 weighted by ionization potential	3D autocorrelations
1800	**TDB08i**	3D Topological distance based descriptors - lag 8 weighted by ionization potential	3D autocorrelations
1801	**TDB09i**	3D Topological distance based descriptors - lag 9 weighted by ionization potential	3D autocorrelations
1802	**TDB10i**	3D Topological distance based descriptors - lag 10 weighted by ionization potential	3D autocorrelations
1803	**TDB01s**	3D Topological distance based descriptors - lag 1 weighted by I-state	3D autocorrelations
1804	**TDB02s**	3D Topological distance based descriptors - lag 2 weighted by I-state	3D autocorrelations
1805	**TDB03s**	3D Topological distance based descriptors - lag 3 weighted by I-state	3D autocorrelations
1806	**TDB04s**	3D Topological distance based descriptors - lag 4 weighted by I-state	3D autocorrelations
1807	**TDB05s**	3D Topological distance based descriptors - lag 5 weighted by I-state	3D autocorrelations
1808	**TDB06s**	3D Topological distance based descriptors - lag 6 weighted by I-state	3D autocorrelations
1809	**TDB07s**	3D Topological distance based descriptors - lag 7 weighted by I-state	3D autocorrelations
1810	**TDB08s**	3D Topological distance based descriptors - lag 8 weighted by I-state	3D autocorrelations

No.	Name	Description	Block
1811	**TDB09s**	3D Topological distance based descriptors - lag 9 weighted by I-state	3D autocorrelations
1812	**TDB10s**	3D Topological distance based descriptors - lag 10 weighted by I-state	3D autocorrelations
1813	**TDB01r**	3D Topological distance based descriptors - lag 1 weighted by covalent radius	3D autocorrelations
1814	**TDB02r**	3D Topological distance based descriptors - lag 2 weighted by covalent radius	3D autocorrelations
1815	**TDB03r**	3D Topological distance based descriptors - lag 3 weighted by covalent radius	3D autocorrelations
1816	**TDB04r**	3D Topological distance based descriptors - lag 4 weighted by covalent radius	3D autocorrelations
1817	**TDB05r**	3D Topological distance based descriptors - lag 5 weighted by covalent radius	3D autocorrelations
1818	**TDB06r**	3D Topological distance based descriptors - lag 6 weighted by covalent radius	3D autocorrelations
1819	**TDB07r**	3D Topological distance based descriptors - lag 7 weighted by covalent radius	3D autocorrelations
1820	**TDB08r**	3D Topological distance based descriptors - lag 8 weighted by covalent radius	3D autocorrelations
1821	**TDB09r**	3D Topological distance based descriptors - lag 9 weighted by covalent radius	3D autocorrelations
1822	**TDB10r**	3D Topological distance based descriptors - lag 10 weighted by covalent radius	3D autocorrelations
1823	**RDF010u**	Radial Distribution Function - 010 / unweighted	RDF descriptors
1824	**RDF015u**	Radial Distribution Function - 015 / unweighted	RDF descriptors
1825	**RDF020u**	Radial Distribution Function - 020 / unweighted	RDF descriptors
1826	**RDF025u**	Radial Distribution Function - 025 / unweighted	RDF descriptors
1827	**RDF030u**	Radial Distribution Function - 030 / unweighted	RDF descriptors
1828	**RDF035u**	Radial Distribution Function - 035 / unweighted	RDF descriptors
1829	**RDF040u**	Radial Distribution Function - 040 / unweighted	RDF descriptors

No.	Name	Description	Block
1830	**RDF045u**	Radial Distribution Function - 045 / unweighted	RDF descriptors
1831	**RDF050u**	Radial Distribution Function - 050 / unweighted	RDF descriptors
1832	**RDF055u**	Radial Distribution Function - 055 / unweighted	RDF descriptors
1833	**RDF060u**	Radial Distribution Function - 060 / unweighted	RDF descriptors
1834	**RDF065u**	Radial Distribution Function - 065 / unweighted	RDF descriptors
1835	**RDF070u**	Radial Distribution Function - 070 / unweighted	RDF descriptors
1836	**RDF075u**	Radial Distribution Function - 075 / unweighted	RDF descriptors
1837	**RDF080u**	Radial Distribution Function - 080 / unweighted	RDF descriptors
1838	**RDF085u**	Radial Distribution Function - 085 / unweighted	RDF descriptors
1839	**RDF090u**	Radial Distribution Function - 090 / unweighted	RDF descriptors
1840	**RDF095u**	Radial Distribution Function - 095 / unweighted	RDF descriptors
1841	**RDF100u**	Radial Distribution Function - 100 / unweighted	RDF descriptors
1842	**RDF105u**	Radial Distribution Function - 105 / unweighted	RDF descriptors
1843	**RDF110u**	Radial Distribution Function - 110 / unweighted	RDF descriptors
1844	**RDF115u**	Radial Distribution Function - 115 / unweighted	RDF descriptors
1845	**RDF120u**	Radial Distribution Function - 120 / unweighted	RDF descriptors
1846	**RDF125u**	Radial Distribution Function - 125 / unweighted	RDF descriptors
1847	**RDF130u**	Radial Distribution Function - 130 / unweighted	RDF descriptors
1848	**RDF135u**	Radial Distribution Function - 135 / unweighted	RDF descriptors

No.	Name	Description	Block
1849	**RDF140u**	Radial Distribution Function - 140 / unweighted	RDF descriptors
1850	**RDF145u**	Radial Distribution Function - 145 / unweighted	RDF descriptors
1851	**RDF150u**	Radial Distribution Function - 150 / unweighted	RDF descriptors
1852	**RDF155u**	Radial Distribution Function - 155 / unweighted	RDF descriptors
1853	**RDF010m**	Radial Distribution Function - 010 / weighted by mass	RDF descriptors
1854	**RDF015m**	Radial Distribution Function - 015 / weighted by mass	RDF descriptors
1855	**RDF020m**	Radial Distribution Function - 020 / weighted by mass	RDF descriptors
1856	**RDF025m**	Radial Distribution Function - 025 / weighted by mass	RDF descriptors
1857	**RDF030m**	Radial Distribution Function - 030 / weighted by mass	RDF descriptors
1858	**RDF035m**	Radial Distribution Function - 035 / weighted by mass	RDF descriptors
1859	**RDF040m**	Radial Distribution Function - 040 / weighted by mass	RDF descriptors
1860	**RDF045m**	Radial Distribution Function - 045 / weighted by mass	RDF descriptors
1861	**RDF050m**	Radial Distribution Function - 050 / weighted by mass	RDF descriptors
1862	**RDF055m**	Radial Distribution Function - 055 / weighted by mass	RDF descriptors
1863	**RDF060m**	Radial Distribution Function - 060 / weighted by mass	RDF descriptors
1864	**RDF065m**	Radial Distribution Function - 065 / weighted by mass	RDF descriptors
1865	**RDF070m**	Radial Distribution Function - 070 / weighted by mass	RDF descriptors
1866	**RDF075m**	Radial Distribution Function - 075 / weighted by mass	RDF descriptors
1867	**RDF080m**	Radial Distribution Function - 080 / weighted by mass	RDF descriptors

No.	Name	Description	Block
1868	**RDF085m**	Radial Distribution Function - 085 / weighted by mass	RDF descriptors
1869	**RDF090m**	Radial Distribution Function - 090 / weighted by mass	RDF descriptors
1870	**RDF095m**	Radial Distribution Function - 095 / weighted by mass	RDF descriptors
1871	**RDF100m**	Radial Distribution Function - 100 / weighted by mass	RDF descriptors
1872	**RDF105m**	Radial Distribution Function - 105 / weighted by mass	RDF descriptors
1873	**RDF110m**	Radial Distribution Function - 110 / weighted by mass	RDF descriptors
1874	**RDF115m**	Radial Distribution Function - 115 / weighted by mass	RDF descriptors
1875	**RDF120m**	Radial Distribution Function - 120 / weighted by mass	RDF descriptors
1876	**RDF125m**	Radial Distribution Function - 125 / weighted by mass	RDF descriptors
1877	**RDF130m**	Radial Distribution Function - 130 / weighted by mass	RDF descriptors
1878	**RDF135m**	Radial Distribution Function - 135 / weighted by mass	RDF descriptors
1879	**RDF140m**	Radial Distribution Function - 140 / weighted by mass	RDF descriptors
1880	**RDF145m**	Radial Distribution Function - 145 / weighted by mass	RDF descriptors
1881	**RDF150m**	Radial Distribution Function - 150 / weighted by mass	RDF descriptors
1882	**RDF155m**	Radial Distribution Function - 155 / weighted by mass	RDF descriptors
1883	**RDF010v**	Radial Distribution Function - 010 / weighted by van der Waals volume	RDF descriptors
1884	**RDF015v**	Radial Distribution Function - 015 / weighted by van der Waals volume	RDF descriptors
1885	**RDF020v**	Radial Distribution Function - 020 / weighted by van der Waals volume	RDF descriptors
1886	**RDF025v**	Radial Distribution Function - 025 / weighted by van der Waals volume	RDF descriptors

No.	Name	Description	Block
1887	**RDF030v**	Radial Distribution Function - 030 / weighted by van der Waals volume	RDF descriptors
1888	**RDF035v**	Radial Distribution Function - 035 / weighted by van der Waals volume	RDF descriptors
1889	**RDF040v**	Radial Distribution Function - 040 / weighted by van der Waals volume	RDF descriptors
1890	**RDF045v**	Radial Distribution Function - 045 / weighted by van der Waals volume	RDF descriptors
1891	**RDF050v**	Radial Distribution Function - 050 / weighted by van der Waals volume	RDF descriptors
1892	**RDF055v**	Radial Distribution Function - 055 / weighted by van der Waals volume	RDF descriptors
1893	**RDF060v**	Radial Distribution Function - 060 / weighted by van der Waals volume	RDF descriptors
1894	**RDF065v**	Radial Distribution Function - 065 / weighted by van der Waals volume	RDF descriptors
1895	**RDF070v**	Radial Distribution Function - 070 / weighted by van der Waals volume	RDF descriptors
1896	**RDF075v**	Radial Distribution Function - 075 / weighted by van der Waals volume	RDF descriptors
1897	**RDF080v**	Radial Distribution Function - 080 / weighted by van der Waals volume	RDF descriptors
1898	**RDF085v**	Radial Distribution Function - 085 / weighted by van der Waals volume	RDF descriptors
1899	**RDF090v**	Radial Distribution Function - 090 / weighted by van der Waals volume	RDF descriptors
1900	**RDF095v**	Radial Distribution Function - 095 / weighted by van der Waals volume	RDF descriptors
1901	**RDF100v**	Radial Distribution Function - 100 / weighted by van der Waals volume	RDF descriptors
1902	**RDF105v**	Radial Distribution Function - 105 / weighted by van der Waals volume	RDF descriptors
1903	**RDF110v**	Radial Distribution Function - 110 / weighted by van der Waals volume	RDF descriptors
1904	**RDF115v**	Radial Distribution Function - 115 / weighted by van der Waals volume	RDF descriptors
1905	**RDF120v**	Radial Distribution Function - 120 / weighted by van der Waals volume	RDF descriptors

No.	Name	Description	Block
1906	**RDF125v**	Radial Distribution Function - 125 / weighted by van der Waals volume	RDF descriptors
1907	**RDF130v**	Radial Distribution Function - 130 / weighted by van der Waals volume	RDF descriptors
1908	**RDF135v**	Radial Distribution Function - 135 / weighted by van der Waals volume	RDF descriptors
1909	**RDF140v**	Radial Distribution Function - 140 / weighted by van der Waals volume	RDF descriptors
1910	**RDF145v**	Radial Distribution Function - 145 / weighted by van der Waals volume	RDF descriptors
1911	**RDF150v**	Radial Distribution Function - 150 / weighted by van der Waals volume	RDF descriptors
1912	**RDF155v**	Radial Distribution Function - 155 / weighted by van der Waals volume	RDF descriptors
1913	**RDF010e**	Radial Distribution Function - 010 / weighted by Sanderson electronegativity	RDF descriptors
1914	**RDF015e**	Radial Distribution Function - 015 / weighted by Sanderson electronegativity	RDF descriptors
1915	**RDF020e**	Radial Distribution Function - 020 / weighted by Sanderson electronegativity	RDF descriptors
1916	**RDF025e**	Radial Distribution Function - 025 / weighted by Sanderson electronegativity	RDF descriptors
1917	**RDF030e**	Radial Distribution Function - 030 / weighted by Sanderson electronegativity	RDF descriptors
1918	**RDF035e**	Radial Distribution Function - 035 / weighted by Sanderson electronegativity	RDF descriptors
1919	**RDF040e**	Radial Distribution Function - 040 / weighted by Sanderson electronegativity	RDF descriptors
1920	**RDF045e**	Radial Distribution Function - 045 / weighted by Sanderson electronegativity	RDF descriptors
1921	**RDF050e**	Radial Distribution Function - 050 / weighted by Sanderson electronegativity	RDF descriptors
1922	**RDF055e**	Radial Distribution Function - 055 / weighted by Sanderson electronegativity	RDF descriptors
1923	**RDF060e**	Radial Distribution Function - 060 / weighted by Sanderson electronegativity	RDF descriptors
1924	**RDF065e**	Radial Distribution Function - 065 / weighted by Sanderson electronegativity	RDF descriptors

No.	Name	Description	Block
1925	**RDF070e**	Radial Distribution Function - 070 / weighted by Sanderson electronegativity	RDF descriptors
1926	**RDF075e**	Radial Distribution Function - 075 / weighted by Sanderson electronegativity	RDF descriptors
1927	**RDF080e**	Radial Distribution Function - 080 / weighted by Sanderson electronegativity	RDF descriptors
1928	**RDF085e**	Radial Distribution Function - 085 / weighted by Sanderson electronegativity	RDF descriptors
1929	**RDF090e**	Radial Distribution Function - 090 / weighted by Sanderson electronegativity	RDF descriptors
1930	**RDF095e**	Radial Distribution Function - 095 / weighted by Sanderson electronegativity	RDF descriptors
1931	**RDF100e**	Radial Distribution Function - 100 / weighted by Sanderson electronegativity	RDF descriptors
1932	**RDF105e**	Radial Distribution Function - 105 / weighted by Sanderson electronegativity	RDF descriptors
1933	**RDF110e**	Radial Distribution Function - 110 / weighted by Sanderson electronegativity	RDF descriptors
1934	**RDF115e**	Radial Distribution Function - 115 / weighted by Sanderson electronegativity	RDF descriptors
1935	**RDF120e**	Radial Distribution Function - 120 / weighted by Sanderson electronegativity	RDF descriptors
1936	**RDF125e**	Radial Distribution Function - 125 / weighted by Sanderson electronegativity	RDF descriptors
1937	**RDF130e**	Radial Distribution Function - 130 / weighted by Sanderson electronegativity	RDF descriptors
1938	**RDF135e**	Radial Distribution Function - 135 / weighted by Sanderson electronegativity	RDF descriptors
1939	**RDF140e**	Radial Distribution Function - 140 / weighted by Sanderson electronegativity	RDF descriptors
1940	**RDF145e**	Radial Distribution Function - 145 / weighted by Sanderson electronegativity	RDF descriptors
1941	**RDF150e**	Radial Distribution Function - 150 / weighted by Sanderson electronegativity	RDF descriptors
1942	**RDF155e**	Radial Distribution Function - 155 / weighted by Sanderson electronegativity	RDF descriptors
1943	**RDF010p**	Radial Distribution Function - 010 / weighted by polarizability	RDF descriptors

No.	Name	Description	Block
1944	**RDF015p**	Radial Distribution Function - 015 / weighted by polarizability	RDF descriptors
1945	**RDF020p**	Radial Distribution Function - 020 / weighted by polarizability	RDF descriptors
1946	**RDF025p**	Radial Distribution Function - 025 / weighted by polarizability	RDF descriptors
1947	**RDF030p**	Radial Distribution Function - 030 / weighted by polarizability	RDF descriptors
1948	**RDF035p**	Radial Distribution Function - 035 / weighted by polarizability	RDF descriptors
1949	**RDF040p**	Radial Distribution Function - 040 / weighted by polarizability	RDF descriptors
1950	**RDF045p**	Radial Distribution Function - 045 / weighted by polarizability	RDF descriptors
1951	**RDF050p**	Radial Distribution Function - 050 / weighted by polarizability	RDF descriptors
1952	**RDF055p**	Radial Distribution Function - 055 / weighted by polarizability	RDF descriptors
1953	**RDF060p**	Radial Distribution Function - 060 / weighted by polarizability	RDF descriptors
1954	**RDF065p**	Radial Distribution Function - 065 / weighted by polarizability	RDF descriptors
1955	**RDF070p**	Radial Distribution Function - 070 / weighted by polarizability	RDF descriptors
1956	**RDF075p**	Radial Distribution Function - 075 / weighted by polarizability	RDF descriptors
1957	**RDF080p**	Radial Distribution Function - 080 / weighted by polarizability	RDF descriptors
1958	**RDF085p**	Radial Distribution Function - 085 / weighted by polarizability	RDF descriptors
1959	**RDF090p**	Radial Distribution Function - 090 / weighted by polarizability	RDF descriptors
1960	**RDF095p**	Radial Distribution Function - 095 / weighted by polarizability	RDF descriptors
1961	**RDF100p**	Radial Distribution Function - 100 / weighted by polarizability	RDF descriptors
1962	**RDF105p**	Radial Distribution Function - 105 / weighted by polarizability	RDF descriptors

No.	Name	Description	Block
1963	**RDF110p**	Radial Distribution Function - 110 / weighted by polarizability	RDF descriptors
1964	**RDF115p**	Radial Distribution Function - 115 / weighted by polarizability	RDF descriptors
1965	**RDF120p**	Radial Distribution Function - 120 / weighted by polarizability	RDF descriptors
1966	**RDF125p**	Radial Distribution Function - 125 / weighted by polarizability	RDF descriptors
1967	**RDF130p**	Radial Distribution Function - 130 / weighted by polarizability	RDF descriptors
1968	**RDF135p**	Radial Distribution Function - 135 / weighted by polarizability	RDF descriptors
1969	**RDF140p**	Radial Distribution Function - 140 / weighted by polarizability	RDF descriptors
1970	**RDF145p**	Radial Distribution Function - 145 / weighted by polarizability	RDF descriptors
1971	**RDF150p**	Radial Distribution Function - 150 / weighted by polarizability	RDF descriptors
1972	**RDF155p**	Radial Distribution Function - 155 / weighted by polarizability	RDF descriptors
1973	**RDF010i**	Radial Distribution Function - 010 / weighted by ionization potential	RDF descriptors
1974	**RDF015i**	Radial Distribution Function - 015 / weighted by ionization potential	RDF descriptors
1975	**RDF020i**	Radial Distribution Function - 020 / weighted by ionization potential	RDF descriptors
1976	**RDF025i**	Radial Distribution Function - 025 / weighted by ionization potential	RDF descriptors
1977	**RDF030i**	Radial Distribution Function - 030 / weighted by ionization potential	RDF descriptors
1978	**RDF035i**	Radial Distribution Function - 035 / weighted by ionization potential	RDF descriptors
1979	**RDF040i**	Radial Distribution Function - 040 / weighted by ionization potential	RDF descriptors
1980	**RDF045i**	Radial Distribution Function - 045 / weighted by ionization potential	RDF descriptors
1981	**RDF050i**	Radial Distribution Function - 050 / weighted by ionization potential	RDF descriptors

No.	Name	Description	Block
1982	**RDF055i**	Radial Distribution Function - 055 / weighted by ionization potential	RDF descriptors
1983	**RDF060i**	Radial Distribution Function - 060 / weighted by ionization potential	RDF descriptors
1984	**RDF065i**	Radial Distribution Function - 065 / weighted by ionization potential	RDF descriptors
1985	**RDF070i**	Radial Distribution Function - 070 / weighted by ionization potential	RDF descriptors
1986	**RDF075i**	Radial Distribution Function - 075 / weighted by ionization potential	RDF descriptors
1987	**RDF080i**	Radial Distribution Function - 080 / weighted by ionization potential	RDF descriptors
1988	**RDF085i**	Radial Distribution Function - 085 / weighted by ionization potential	RDF descriptors
1989	**RDF090i**	Radial Distribution Function - 090 / weighted by ionization potential	RDF descriptors
1990	**RDF095i**	Radial Distribution Function - 095 / weighted by ionization potential	RDF descriptors
1991	**RDF100i**	Radial Distribution Function - 100 / weighted by ionization potential	RDF descriptors
1992	**RDF105i**	Radial Distribution Function - 105 / weighted by ionization potential	RDF descriptors
1993	**RDF110i**	Radial Distribution Function - 110 / weighted by ionization potential	RDF descriptors
1994	**RDF115i**	Radial Distribution Function - 115 / weighted by ionization potential	RDF descriptors
1995	**RDF120i**	Radial Distribution Function - 120 / weighted by ionization potential	RDF descriptors
1996	**RDF125i**	Radial Distribution Function - 125 / weighted by ionization potential	RDF descriptors
1997	**RDF130i**	Radial Distribution Function - 130 / weighted by ionization potential	RDF descriptors
1998	**RDF135i**	Radial Distribution Function - 135 / weighted by ionization potential	RDF descriptors
1999	**RDF140i**	Radial Distribution Function - 140 / weighted by ionization potential	RDF descriptors
2000	**RDF145i**	Radial Distribution Function - 145 / weighted by ionization potential	RDF descriptors

No.	Name	Description	Block
2001	**RDF150i**	Radial Distribution Function - 150 / weighted by ionization potential	RDF descriptors
2002	**RDF155i**	Radial Distribution Function - 155 / weighted by ionization potential	RDF descriptors
2003	**RDF010s**	Radial Distribution Function - 010 / weighted by I-state	RDF descriptors
2004	**RDF015s**	Radial Distribution Function - 015 / weighted by I-state	RDF descriptors
2005	**RDF020s**	Radial Distribution Function - 020 / weighted by I-state	RDF descriptors
2006	**RDF025s**	Radial Distribution Function - 025 / weighted by I-state	RDF descriptors
2007	**RDF030s**	Radial Distribution Function - 030 / weighted by I-state	RDF descriptors
2008	**RDF035s**	Radial Distribution Function - 035 / weighted by I-state	RDF descriptors
2009	**RDF040s**	Radial Distribution Function - 040 / weighted by I-state	RDF descriptors
2010	**RDF045s**	Radial Distribution Function - 045 / weighted by I-state	RDF descriptors
2011	**RDF050s**	Radial Distribution Function - 050 / weighted by I-state	RDF descriptors
2012	**RDF055s**	Radial Distribution Function - 055 / weighted by I-state	RDF descriptors
2013	**RDF060s**	Radial Distribution Function - 060 / weighted by I-state	RDF descriptors
2014	**RDF065s**	Radial Distribution Function - 065 / weighted by I-state	RDF descriptors
2015	**RDF070s**	Radial Distribution Function - 070 / weighted by I-state	RDF descriptors
2016	**RDF075s**	Radial Distribution Function - 075 / weighted by I-state	RDF descriptors
2017	**RDF080s**	Radial Distribution Function - 080 / weighted by I-state	RDF descriptors
2018	**RDF085s**	Radial Distribution Function - 085 / weighted by I-state	RDF descriptors
2019	**RDF090s**	Radial Distribution Function - 090 / weighted by I-state	RDF descriptors

No.	Name	Description	Block
2020	**RDF095s**	Radial Distribution Function - 095 / weighted by I-state	RDF descriptors
2021	**RDF100s**	Radial Distribution Function - 100 / weighted by I-state	RDF descriptors
2022	**RDF105s**	Radial Distribution Function - 105 / weighted by I-state	RDF descriptors
2023	**RDF110s**	Radial Distribution Function - 110 / weighted by I-state	RDF descriptors
2024	**RDF115s**	Radial Distribution Function - 115 / weighted by I-state	RDF descriptors
2025	**RDF120s**	Radial Distribution Function - 120 / weighted by I-state	RDF descriptors
2026	**RDF125s**	Radial Distribution Function - 125 / weighted by I-state	RDF descriptors
2027	**RDF130s**	Radial Distribution Function - 130 / weighted by I-state	RDF descriptors
2028	**RDF135s**	Radial Distribution Function - 135 / weighted by I-state	RDF descriptors
2029	**RDF140s**	Radial Distribution Function - 140 / weighted by I-state	RDF descriptors
2030	**RDF145s**	Radial Distribution Function - 145 / weighted by I-state	RDF descriptors
2031	**RDF150s**	Radial Distribution Function - 150 / weighted by I-state	RDF descriptors
2032	**RDF155s**	Radial Distribution Function - 155 / weighted by I-state	RDF descriptors
2033	**Mor01u**	signal 01 / unweighted	3D-MoRSE descriptors
2034	**Mor02u**	signal 02 / unweighted	3D-MoRSE descriptors
2035	**Mor03u**	signal 03 / unweighted	3D-MoRSE descriptors
2036	**Mor04u**	signal 04 / unweighted	3D-MoRSE descriptors
2037	**Mor05u**	signal 05 / unweighted	3D-MoRSE descriptors
2038	**Mor06u**	signal 06 / unweighted	3D-MoRSE descriptors

No.	Name	Description	Block
2039	**Mor07u**	signal 07 / unweighted	3D-MoRSE descriptors
2040	**Mor08u**	signal 08 / unweighted	3D-MoRSE descriptors
2041	**Mor09u**	signal 09 / unweighted	3D-MoRSE descriptors
2042	**Mor10u**	signal 10 / unweighted	3D-MoRSE descriptors
2043	**Mor11u**	signal 11 / unweighted	3D-MoRSE descriptors
2044	**Mor12u**	signal 12 / unweighted	3D-MoRSE descriptors
2045	**Mor13u**	signal 13 / unweighted	3D-MoRSE descriptors
2046	**Mor14u**	signal 14 / unweighted	3D-MoRSE descriptors
2047	**Mor15u**	signal 15 / unweighted	3D-MoRSE descriptors
2048	**Mor16u**	signal 16 / unweighted	3D-MoRSE descriptors
2049	**Mor17u**	signal 17 / unweighted	3D-MoRSE descriptors
2050	**Mor18u**	signal 18 / unweighted	3D-MoRSE descriptors
2051	**Mor19u**	signal 19 / unweighted	3D-MoRSE descriptors
2052	**Mor20u**	signal 20 / unweighted	3D-MoRSE descriptors
2053	**Mor21u**	signal 21 / unweighted	3D-MoRSE descriptors
2054	**Mor22u**	signal 22 / unweighted	3D-MoRSE descriptors
2055	**Mor23u**	signal 23 / unweighted	3D-MoRSE descriptors
2056	**Mor24u**	signal 24 / unweighted	3D-MoRSE descriptors
2057	**Mor25u**	signal 25 / unweighted	3D-MoRSE descriptors

No.	Name	Description	Block
2058	**Mor26u**	signal 26 / unweighted	3D-MoRSE descriptors
2059	**Mor27u**	signal 27 / unweighted	3D-MoRSE descriptors
2060	**Mor28u**	signal 28 / unweighted	3D-MoRSE descriptors
2061	**Mor29u**	signal 29 / unweighted	3D-MoRSE descriptors
2062	**Mor30u**	signal 30 / unweighted	3D-MoRSE descriptors
2063	**Mor31u**	signal 31 / unweighted	3D-MoRSE descriptors
2064	**Mor32u**	signal 32 / unweighted	3D-MoRSE descriptors
2065	**Mor01m**	signal 01 / weighted by mass	3D-MoRSE descriptors
2066	**Mor02m**	signal 02 / weighted by mass	3D-MoRSE descriptors
2067	**Mor03m**	signal 03 / weighted by mass	3D-MoRSE descriptors
2068	**Mor04m**	signal 04 / weighted by mass	3D-MoRSE descriptors
2069	**Mor05m**	signal 05 / weighted by mass	3D-MoRSE descriptors
2070	**Mor06m**	signal 06 / weighted by mass	3D-MoRSE descriptors
2071	**Mor07m**	signal 07 / weighted by mass	3D-MoRSE descriptors
2072	**Mor08m**	signal 08 / weighted by mass	3D-MoRSE descriptors
2073	**Mor09m**	signal 09 / weighted by mass	3D-MoRSE descriptors
2074	**Mor10m**	signal 10 / weighted by mass	3D-MoRSE descriptors
2075	**Mor11m**	signal 11 / weighted by mass	3D-MoRSE descriptors
2076	**Mor12m**	signal 12 / weighted by mass	3D-MoRSE descriptors

No.	Name	Description	Block
2077	**Mor13m**	signal 13 / weighted by mass	3D-MoRSE descriptors
2078	**Mor14m**	signal 14 / weighted by mass	3D-MoRSE descriptors
2079	**Mor15m**	signal 15 / weighted by mass	3D-MoRSE descriptors
2080	**Mor16m**	signal 16 / weighted by mass	3D-MoRSE descriptors
2081	**Mor17m**	signal 17 / weighted by mass	3D-MoRSE descriptors
2082	**Mor18m**	signal 18 / weighted by mass	3D-MoRSE descriptors
2083	**Mor19m**	signal 19 / weighted by mass	3D-MoRSE descriptors
2084	**Mor20m**	signal 20 / weighted by mass	3D-MoRSE descriptors
2085	**Mor21m**	signal 21 / weighted by mass	3D-MoRSE descriptors
2086	**Mor22m**	signal 22 / weighted by mass	3D-MoRSE descriptors
2087	**Mor23m**	signal 23 / weighted by mass	3D-MoRSE descriptors
2088	**Mor24m**	signal 24 / weighted by mass	3D-MoRSE descriptors
2089	**Mor25m**	signal 25 / weighted by mass	3D-MoRSE descriptors
2090	**Mor26m**	signal 26 / weighted by mass	3D-MoRSE descriptors
2091	**Mor27m**	signal 27 / weighted by mass	3D-MoRSE descriptors
2092	**Mor28m**	signal 28 / weighted by mass	3D-MoRSE descriptors
2093	**Mor29m**	signal 29 / weighted by mass	3D-MoRSE descriptors
2094	**Mor30m**	signal 30 / weighted by mass	3D-MoRSE descriptors
2095	**Mor31m**	signal 31 / weighted by mass	3D-MoRSE descriptors

No.	Name	Description	Block
2096	**Mor32m**	signal 32 / weighted by mass	3D-MoRSE descriptors
2097	**Mor01v**	signal 01 / weighted by van der Waals volume	3D-MoRSE descriptors
2098	**Mor02v**	signal 02 / weighted by van der Waals volume	3D-MoRSE descriptors
2099	**Mor03v**	signal 03 / weighted by van der Waals volume	3D-MoRSE descriptors
2100	**Mor04v**	signal 04 / weighted by van der Waals volume	3D-MoRSE descriptors
2101	**Mor05v**	signal 05 / weighted by van der Waals volume	3D-MoRSE descriptors
2102	**Mor06v**	signal 06 / weighted by van der Waals volume	3D-MoRSE descriptors
2103	**Mor07v**	signal 07 / weighted by van der Waals volume	3D-MoRSE descriptors
2104	**Mor08v**	signal 08 / weighted by van der Waals volume	3D-MoRSE descriptors
2105	**Mor09v**	signal 09 / weighted by van der Waals volume	3D-MoRSE descriptors
2106	**Mor10v**	signal 10 / weighted by van der Waals volume	3D-MoRSE descriptors
2107	**Mor11v**	signal 11 / weighted by van der Waals volume	3D-MoRSE descriptors
2108	**Mor12v**	signal 12 / weighted by van der Waals volume	3D-MoRSE descriptors
2109	**Mor13v**	signal 13 / weighted by van der Waals volume	3D-MoRSE descriptors
2110	**Mor14v**	signal 14 / weighted by van der Waals volume	3D-MoRSE descriptors
2111	**Mor15v**	signal 15 / weighted by van der Waals volume	3D-MoRSE descriptors
2112	**Mor16v**	signal 16 / weighted by van der Waals volume	3D-MoRSE descriptors
2113	**Mor17v**	signal 17 / weighted by van der Waals volume	3D-MoRSE descriptors
2114	**Mor18v**	signal 18 / weighted by van der Waals volume	3D-MoRSE descriptors

No.	Name	Description	Block
2115	**Mor19v**	signal 19 / weighted by van der Waals volume	3D-MoRSE descriptors
2116	**Mor20v**	signal 20 / weighted by van der Waals volume	3D-MoRSE descriptors
2117	**Mor21v**	signal 21 / weighted by van der Waals volume	3D-MoRSE descriptors
2118	**Mor22v**	signal 22 / weighted by van der Waals volume	3D-MoRSE descriptors
2119	**Mor23v**	signal 23 / weighted by van der Waals volume	3D-MoRSE descriptors
2120	**Mor24v**	signal 24 / weighted by van der Waals volume	3D-MoRSE descriptors
2121	**Mor25v**	signal 25 / weighted by van der Waals volume	3D-MoRSE descriptors
2122	**Mor26v**	signal 26 / weighted by van der Waals volume	3D-MoRSE descriptors
2123	**Mor27v**	signal 27 / weighted by van der Waals volume	3D-MoRSE descriptors
2124	**Mor28v**	signal 28 / weighted by van der Waals volume	3D-MoRSE descriptors
2125	**Mor29v**	signal 29 / weighted by van der Waals volume	3D-MoRSE descriptors
2126	**Mor30v**	signal 30 / weighted by van der Waals volume	3D-MoRSE descriptors
2127	**Mor31v**	signal 31 / weighted by van der Waals volume	3D-MoRSE descriptors
2128	**Mor32v**	signal 32 / weighted by van der Waals volume	3D-MoRSE descriptors
2129	**Mor01e**	signal 01 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2130	**Mor02e**	signal 02 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2131	**Mor03e**	signal 03 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2132	**Mor04e**	signal 04 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2133	**Mor05e**	signal 05 / weighted by Sanderson electronegativity	3D-MoRSE descriptors

No.	Name	Description	Block
2134	**Mor06e**	signal 06 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2135	**Mor07e**	signal 07 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2136	**Mor08e**	signal 08 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2137	**Mor09e**	signal 09 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2138	**Mor10e**	signal 10 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2139	**Mor11e**	signal 11 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2140	**Mor12e**	signal 12 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2141	**Mor13e**	signal 13 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2142	**Mor14e**	signal 14 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2143	**Mor15e**	signal 15 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2144	**Mor16e**	signal 16 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2145	**Mor17e**	signal 17 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2146	**Mor18e**	signal 18 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2147	**Mor19e**	signal 19 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2148	**Mor20e**	signal 20 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2149	**Mor21e**	signal 21 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2150	**Mor22e**	signal 22 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2151	**Mor23e**	signal 23 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2152	**Mor24e**	signal 24 / weighted by Sanderson electronegativity	3D-MoRSE descriptors

No.	Name	Description	Block
2153	**Mor25e**	signal 25 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2154	**Mor26e**	signal 26 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2155	**Mor27e**	signal 27 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2156	**Mor28e**	signal 28 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2157	**Mor29e**	signal 29 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2158	**Mor30e**	signal 30 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2159	**Mor31e**	signal 31 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2160	**Mor32e**	signal 32 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2161	**Mor01p**	signal 01 / weighted by polarizability	3D-MoRSE descriptors
2162	**Mor02p**	signal 02 / weighted by polarizability	3D-MoRSE descriptors
2163	**Mor03p**	signal 03 / weighted by polarizability	3D-MoRSE descriptors
2164	**Mor04p**	signal 04 / weighted by polarizability	3D-MoRSE descriptors
2165	**Mor05p**	signal 05 / weighted by polarizability	3D-MoRSE descriptors
2166	**Mor06p**	signal 06 / weighted by polarizability	3D-MoRSE descriptors
2167	**Mor07p**	signal 07 / weighted by polarizability	3D-MoRSE descriptors
2168	**Mor08p**	signal 08 / weighted by polarizability	3D-MoRSE descriptors
2169	**Mor09p**	signal 09 / weighted by polarizability	3D-MoRSE descriptors
2170	**Mor10p**	signal 10 / weighted by polarizability	3D-MoRSE descriptors
2171	**Mor11p**	signal 11 / weighted by polarizability	3D-MoRSE descriptors

No.	Name	Description	Block
2172	**Mor12p**	signal 12 / weighted by polarizability	3D-MoRSE descriptors
2173	**Mor13p**	signal 13 / weighted by polarizability	3D-MoRSE descriptors
2174	**Mor14p**	signal 14 / weighted by polarizability	3D-MoRSE descriptors
2175	**Mor15p**	signal 15 / weighted by polarizability	3D-MoRSE descriptors
2176	**Mor16p**	signal 16 / weighted by polarizability	3D-MoRSE descriptors
2177	**Mor17p**	signal 17 / weighted by polarizability	3D-MoRSE descriptors
2178	**Mor18p**	signal 18 / weighted by polarizability	3D-MoRSE descriptors
2179	**Mor19p**	signal 19 / weighted by polarizability	3D-MoRSE descriptors
2180	**Mor20p**	signal 20 / weighted by polarizability	3D-MoRSE descriptors
2181	**Mor21p**	signal 21 / weighted by polarizability	3D-MoRSE descriptors
2182	**Mor22p**	signal 22 / weighted by polarizability	3D-MoRSE descriptors
2183	**Mor23p**	signal 23 / weighted by polarizability	3D-MoRSE descriptors
2184	**Mor24p**	signal 24 / weighted by polarizability	3D-MoRSE descriptors
2185	**Mor25p**	signal 25 / weighted by polarizability	3D-MoRSE descriptors
2186	**Mor26p**	signal 26 / weighted by polarizability	3D-MoRSE descriptors
2187	**Mor27p**	signal 27 / weighted by polarizability	3D-MoRSE descriptors
2188	**Mor28p**	signal 28 / weighted by polarizability	3D-MoRSE descriptors
2189	**Mor29p**	signal 29 / weighted by polarizability	3D-MoRSE descriptors
2190	**Mor30p**	signal 30 / weighted by polarizability	3D-MoRSE descriptors

No.	Name	Description	Block
2191	**Mor31p**	signal 31 / weighted by polarizability	3D-MoRSE descriptors
2192	**Mor32p**	signal 32 / weighted by polarizability	3D-MoRSE descriptors
2193	**Mor01i**	signal 01 / weighted by ionization potential	3D-MoRSE descriptors
2194	**Mor02i**	signal 02 / weighted by ionization potential	3D-MoRSE descriptors
2195	**Mor03i**	signal 03 / weighted by ionization potential	3D-MoRSE descriptors
2196	**Mor04i**	signal 04 / weighted by ionization potential	3D-MoRSE descriptors
2197	**Mor05i**	signal 05 / weighted by ionization potential	3D-MoRSE descriptors
2198	**Mor06i**	signal 06 / weighted by ionization potential	3D-MoRSE descriptors
2199	**Mor07i**	signal 07 / weighted by ionization potential	3D-MoRSE descriptors
2200	**Mor08i**	signal 08 / weighted by ionization potential	3D-MoRSE descriptors
2201	**Mor09i**	signal 09 / weighted by ionization potential	3D-MoRSE descriptors
2202	**Mor10i**	signal 10 / weighted by ionization potential	3D-MoRSE descriptors
2203	**Mor11i**	signal 11 / weighted by ionization potential	3D-MoRSE descriptors
2204	**Mor12i**	signal 12 / weighted by ionization potential	3D-MoRSE descriptors
2205	**Mor13i**	signal 13 / weighted by ionization potential	3D-MoRSE descriptors
2206	**Mor14i**	signal 14 / weighted by ionization potential	3D-MoRSE descriptors
2207	**Mor15i**	signal 15 / weighted by ionization potential	3D-MoRSE descriptors
2208	**Mor16i**	signal 16 / weighted by ionization potential	3D-MoRSE descriptors
2209	**Mor17i**	signal 17 / weighted by ionization potential	3D-MoRSE descriptors

No.	Name	Description	Block
2210	**Mor18i**	signal 18 / weighted by ionization potential	3D-MoRSE descriptors
2211	**Mor19i**	signal 19 / weighted by ionization potential	3D-MoRSE descriptors
2212	**Mor20i**	signal 20 / weighted by ionization potential	3D-MoRSE descriptors
2213	**Mor21i**	signal 21 / weighted by ionization potential	3D-MoRSE descriptors
2214	**Mor22i**	signal 22 / weighted by ionization potential	3D-MoRSE descriptors
2215	**Mor23i**	signal 23 / weighted by ionization potential	3D-MoRSE descriptors
2216	**Mor24i**	signal 24 / weighted by ionization potential	3D-MoRSE descriptors
2217	**Mor25i**	signal 25 / weighted by ionization potential	3D-MoRSE descriptors
2218	**Mor26i**	signal 26 / weighted by ionization potential	3D-MoRSE descriptors
2219	**Mor27i**	signal 27 / weighted by ionization potential	3D-MoRSE descriptors
2220	**Mor28i**	signal 28 / weighted by ionization potential	3D-MoRSE descriptors
2221	**Mor29i**	signal 29 / weighted by ionization potential	3D-MoRSE descriptors
2222	**Mor30i**	signal 30 / weighted by ionization potential	3D-MoRSE descriptors
2223	**Mor31i**	signal 31 / weighted by ionization potential	3D-MoRSE descriptors
2224	**Mor32i**	signal 32 / weighted by ionization potential	3D-MoRSE descriptors
2225	**Mor01s**	signal 01 / weighted by I-state	3D-MoRSE descriptors
2226	**Mor02s**	signal 02 / weighted by I-state	3D-MoRSE descriptors
2227	**Mor03s**	signal 03 / weighted by I-state	3D-MoRSE descriptors
2228	**Mor04s**	signal 04 / weighted by I-state	3D-MoRSE descriptors

No.	Name	Description	Block
2229	**Mor05s**	signal 05 / weighted by I-state	3D-MoRSE descriptors
2230	**Mor06s**	signal 06 / weighted by I-state	3D-MoRSE descriptors
2231	**Mor07s**	signal 07 / weighted by I-state	3D-MoRSE descriptors
2232	**Mor08s**	signal 08 / weighted by I-state	3D-MoRSE descriptors
2233	**Mor09s**	signal 09 / weighted by I-state	3D-MoRSE descriptors
2234	**Mor10s**	signal 10 / weighted by I-state	3D-MoRSE descriptors
2235	**Mor11s**	signal 11 / weighted by I-state	3D-MoRSE descriptors
2236	**Mor12s**	signal 12 / weighted by I-state	3D-MoRSE descriptors
2237	**Mor13s**	signal 13 / weighted by I-state	3D-MoRSE descriptors
2238	**Mor14s**	signal 14 / weighted by I-state	3D-MoRSE descriptors
2239	**Mor15s**	signal 15 / weighted by I-state	3D-MoRSE descriptors
2240	**Mor16s**	signal 16 / weighted by I-state	3D-MoRSE descriptors
2241	**Mor17s**	signal 17 / weighted by I-state	3D-MoRSE descriptors
2242	**Mor18s**	signal 18 / weighted by I-state	3D-MoRSE descriptors
2243	**Mor19s**	signal 19 / weighted by I-state	3D-MoRSE descriptors
2244	**Mor20s**	signal 20 / weighted by I-state	3D-MoRSE descriptors
2245	**Mor21s**	signal 21 / weighted by I-state	3D-MoRSE descriptors
2246	**Mor22s**	signal 22 / weighted by I-state	3D-MoRSE descriptors
2247	**Mor23s**	signal 23 / weighted by I-state	3D-MoRSE descriptors

No.	Name	Description	Block
2248	**Mor24s**	signal 24 / weighted by I-state	3D-MoRSE descriptors
2249	**Mor25s**	signal 25 / weighted by I-state	3D-MoRSE descriptors
2250	**Mor26s**	signal 26 / weighted by I-state	3D-MoRSE descriptors
2251	**Mor27s**	signal 27 / weighted by I-state	3D-MoRSE descriptors
2252	**Mor28s**	signal 28 / weighted by I-state	3D-MoRSE descriptors
2253	**Mor29s**	signal 29 / weighted by I-state	3D-MoRSE descriptors
2254	**Mor30s**	signal 30 / weighted by I-state	3D-MoRSE descriptors
2255	**Mor31s**	signal 31 / weighted by I-state	3D-MoRSE descriptors
2256	**Mor32s**	signal 32 / weighted by I-state	3D-MoRSE descriptors
2257	**L1u**	1st component size directional WHIM index / unweighted	WHIM descriptors
2258	**L2u**	2nd component size directional WHIM index / unweighted	WHIM descriptors
2259	**L3u**	3rd component size directional WHIM index / unweighted	WHIM descriptors
2260	**P1u**	1st component shape directional WHIM index / unweighted	WHIM descriptors
2261	**P2u**	2nd component shape directional WHIM index / unweighted	WHIM descriptors
2262	**G1u**	1st component symmetry directional WHIM index / unweighted	WHIM descriptors
2263	**G2u**	2nd component symmetry directional WHIM index / unweighted	WHIM descriptors
2264	**G3u**	3rd component symmetry directional WHIM index / unweighted	WHIM descriptors
2265	**E1u**	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
2266	**E2u**	2nd component accessibility directional WHIM index / unweighted	WHIM descriptors

No.	Name	Description	Block
2267	**E3u**	3rd component accessibility directional WHIM index / unweighted	WHIM descriptors
2268	**L1m**	1st component size directional WHIM index / weighted by mass	WHIM descriptors
2269	**L2m**	2nd component size directional WHIM index / weighted by mass	WHIM descriptors
2270	**L3m**	3rd component size directional WHIM index / weighted by mass	WHIM descriptors
2271	**P1m**	1st component shape directional WHIM index / weighted by mass	WHIM descriptors
2272	**P2m**	2nd component shape directional WHIM index / weighted by mass	WHIM descriptors
2273	**G1m**	1st component symmetry directional WHIM index / weighted by mass	WHIM descriptors
2274	**G2m**	2nd component symmetry directional WHIM index / weighted by mass	WHIM descriptors
2275	**G3m**	3rd component symmetry directional WHIM index / weighted by mass	WHIM descriptors
2276	**E1m**	1st component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2277	**E2m**	2nd component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2278	**E3m**	3rd component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2279	**L1v**	1st component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2280	**L2v**	2nd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2281	**L3v**	3rd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2282	**P1v**	1st component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2283	**P2v**	2nd component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2284	**G1v**	1st component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2285	**G2v**	2nd component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors

No.	Name	Description	Block
2286	**G3v**	3rd component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2287	**E1v**	1st component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2288	**E2v**	2nd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2289	**E3v**	3rd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2290	**L1e**	1st component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2291	**L2e**	2nd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2292	**L3e**	3rd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2293	**P1e**	1st component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2294	**P2e**	2nd component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2295	**G1e**	1st component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2296	**G2e**	2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2297	**G3e**	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2298	**E1e**	1st component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2299	**E2e**	2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2300	**E3e**	3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2301	**L1p**	1st component size directional WHIM index / weighted by polarizability	WHIM descriptors
2302	**L2p**	2nd component size directional WHIM index / weighted by polarizability	WHIM descriptors
2303	**L3p**	3rd component size directional WHIM index / weighted by polarizability	WHIM descriptors
2304	**P1p**	1st component shape directional WHIM index / weighted by polarizability	WHIM descriptors

No.	Name	Description	Block
2305	**P2p**	2nd component shape directional WHIM index / weighted by polarizability	WHIM descriptors
2306	**G1p**	1st component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2307	**G2p**	2nd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2308	**G3p**	3rd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2309	**E1p**	1st component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2310	**E2p**	2nd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2311	**E3p**	3rd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2312	**L1i**	1st component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2313	**L2i**	2nd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2314	**L3i**	3rd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2315	**P1i**	1st component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
2316	**P2i**	2nd component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
2317	**G1i**	1st component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2318	**G2i**	2nd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2319	**G3i**	3rd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2320	**E1i**	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2321	**E2i**	2nd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2322	**E3i**	3rd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2323	**L1s**	1st component size directional WHIM index / weighted by I-state	WHIM descriptors

No.	Name	Description	Block
2324	**L2s**	2nd component size directional WHIM index / weighted by I-state	WHIM descriptors
2325	**L3s**	3rd component size directional WHIM index / weighted by I-state	WHIM descriptors
2326	**P1s**	1st component shape directional WHIM index / weighted by I-state	WHIM descriptors
2327	**P2s**	2nd component shape directional WHIM index / weighted by I-state	WHIM descriptors
2328	**G1s**	1st component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2329	**G2s**	2nd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2330	**G3s**	3rd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2331	**E1s**	1st component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2332	**E2s**	2nd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2333	**E3s**	3rd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2334	**Tu**	T total size index / unweighted	WHIM descriptors
2335	**Tm**	T total size index / weighted by mass	WHIM descriptors
2336	**Tv**	T total size index / weighted by van der Waals volume	WHIM descriptors
2337	**Te**	T total size index / weighted by Sanderson electronegativity	WHIM descriptors
2338	**Tp**	T total size index / weighted by polarizability	WHIM descriptors
2339	**Ti**	T total size index / weighted by ionization potential	WHIM descriptors
2340	**Ts**	T total size index / weighted by I-state	WHIM descriptors
2341	**Au**	A total size index / unweighted	WHIM descriptors
2342	**Am**	A total size index / weighted by mass	WHIM descriptors

No.	Name	Description	Block
2343	**Av**	A total size index / weighted by van der Waals volume	WHIM descriptors
2344	**Ae**	A total size index / weighted by Sanderson electronegativity	WHIM descriptors
2345	**Ap**	A total size index / weighted by polarizability	WHIM descriptors
2346	**Ai**	A total size index / weighted by ionization potential	WHIM descriptors
2347	**As**	A total size index / weighted by I-state	WHIM descriptors
2348	**Gu**	total symmetry index / unweighted	WHIM descriptors
2349	**Gm**	total symmetry index / weighted by mass	WHIM descriptors
2350	**Ku**	K global shape index / unweighted	WHIM descriptors
2351	**Km**	K global shape index / weighted by mass	WHIM descriptors
2352	**Kv**	K global shape index / weighted by van der Waals volume	WHIM descriptors
2353	**Ke**	K global shape index / weighted by Sanderson electronegativity	WHIM descriptors
2354	**Kp**	K global shape index / weighted by polarizability	WHIM descriptors
2355	**Ki**	K global shape index / weighted by ionization potential	WHIM descriptors
2356	**Ks**	K global shape index / weighted by I-state	WHIM descriptors
2357	**Du**	D total accessibility index / unweighted	WHIM descriptors
2358	**Dm**	D total accessibility index / weighted by mass	WHIM descriptors
2359	**Dv**	D total accessibility index / weighted by van der Waals volume	WHIM descriptors
2360	**De**	D total accessibility index / weighted by Sanderson electronegativity	WHIM descriptors
2361	**Dp**	D total accessibility index / weighted by polarizability	WHIM descriptors

No.	Name	Description	Block
2362	**Di**	D total accessibility index / weighted by ionization potential	WHIM descriptors
2363	**Ds**	D total accessibility index / weighted by I-state	WHIM descriptors
2364	**Vu**	V total size index / unweighted	WHIM descriptors
2365	**Vm**	V total size index / weighted by mass	WHIM descriptors
2366	**Vv**	V total size index / weighted by van der Waals volume	WHIM descriptors
2367	**Ve**	V total size index / weighted by Sanderson electronegativity	WHIM descriptors
2368	**Vp**	V total size index / weighted by polarizability	WHIM descriptors
2369	**Vi**	V total size index / weighted by ionization potential	WHIM descriptors
2370	**Vs**	V total size index / weighted by I-state	WHIM descriptors
2371	**ITH**	total information content on the leverage equality	GETAWAY descriptors
2372	**ISH**	standardized information content on the leverage equality	GETAWAY descriptors
2373	**HIC**	mean information content on the leverage magnitude	GETAWAY descriptors
2374	**HGM**	geometric mean on the leverage magnitude	GETAWAY descriptors
2375	**H0u**	H autocorrelation of lag 0 / unweighted	GETAWAY descriptors
2376	**H1u**	H autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2377	**H2u**	H autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2378	**H3u**	H autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2379	**H4u**	H autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2380	**H5u**	H autocorrelation of lag 5 / unweighted	GETAWAY descriptors

No.	Name	Description	Block
2381	**H6u**	H autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2382	**H7u**	H autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2383	**H8u**	H autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2384	**HTu**	H total index / unweighted	GETAWAY descriptors
2385	**HATS0u**	leverage-weighted autocorrelation of lag 0 / unweighted	GETAWAY descriptors
2386	**HATS1u**	leverage-weighted autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2387	**HATS2u**	leverage-weighted autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2388	**HATS3u**	leverage-weighted autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2389	**HATS4u**	leverage-weighted autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2390	**HATS5u**	leverage-weighted autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2391	**HATS6u**	leverage-weighted autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2392	**HATS7u**	leverage-weighted autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2393	**HATS8u**	leverage-weighted autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2394	**HATSu**	leverage-weighted total index / unweighted	GETAWAY descriptors
2395	**H0m**	H autocorrelation of lag 0 / weighted by mass	GETAWAY descriptors
2396	**H1m**	H autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2397	**H2m**	H autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2398	**H3m**	H autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2399	**H4m**	H autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors

No.	Name	Description	Block
2400	**H5m**	H autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2401	**H6m**	H autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2402	**H7m**	H autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors
2403	**H8m**	H autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2404	**HTm**	H total index / weighted by mass	GETAWAY descriptors
2405	**HATS0m**	leverage-weighted autocorrelation of lag 0 / weighted by mass	GETAWAY descriptors
2406	**HATS1m**	leverage-weighted autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2407	**HATS2m**	leverage-weighted autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2408	**HATS3m**	leverage-weighted autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2409	**HATS4m**	leverage-weighted autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors
2410	**HATS5m**	leverage-weighted autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2411	**HATS6m**	leverage-weighted autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2412	**HATS7m**	leverage-weighted autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors
2413	**HATS8m**	leverage-weighted autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2414	**HATSm**	leverage-weighted total index / weighted by mass	GETAWAY descriptors
2415	**H0v**	H autocorrelation of lag 0 / weighted by van der Waals volume	GETAWAY descriptors
2416	**H1v**	H autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2417	**H2v**	H autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2418	**H3v**	H autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors

No.	Name	Description	Block
2419	**H4v**	H autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2420	**H5v**	H autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2421	**H6v**	H autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2422	**H7v**	H autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2423	**H8v**	H autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors
2424	**HTv**	H total index / weighted by van der Waals volume	GETAWAY descriptors
2425	**HATS0v**	leverage-weighted autocorrelation of lag 0 / weighted by van der Waals volume	GETAWAY descriptors
2426	**HATS1v**	leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2427	**HATS2v**	leverage-weighted autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2428	**HATS3v**	leverage-weighted autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors
2429	**HATS4v**	leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2430	**HATS5v**	leverage-weighted autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2431	**HATS6v**	leverage-weighted autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2432	**HATS7v**	leverage-weighted autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2433	**HATS8v**	leverage-weighted autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors
2434	**HATSv**	leverage-weighted total index / weighted by van der Waals volume	GETAWAY descriptors
2435	**H0e**	H autocorrelation of lag 0 / weighted by Sanderson electronegativity	GETAWAY descriptors
2436	**H1e**	H autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2437	**H2e**	H autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors

No.	Name	Description	Block
2438	**H3e**	H autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors
2439	**H4e**	H autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors
2440	**H5e**	H autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2441	**H6e**	H autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2442	**H7e**	H autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2443	**H8e**	H autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2444	**HTe**	H total index / weighted by Sanderson electronegativity	GETAWAY descriptors
2445	**HATS0e**	leverage-weighted autocorrelation of lag 0 / weighted by Sanderson electronegativity	GETAWAY descriptors
2446	**HATS1e**	leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2447	**HATS2e**	leverage-weighted autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors
2448	**HATS3e**	leverage-weighted autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors
2449	**HATS4e**	leverage-weighted autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors
2450	**HATS5e**	leverage-weighted autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2451	**HATS6e**	leverage-weighted autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2452	**HATS7e**	leverage-weighted autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2453	**HATS8e**	leverage-weighted autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2454	**HATSe**	leverage-weighted total index / weighted by Sanderson electronegativity	GETAWAY descriptors
2455	**H0p**	H autocorrelation of lag 0 / weighted by polarizability	GETAWAY descriptors
2456	**H1p**	H autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors

No.	Name	Description	Block
2457	**H2p**	H autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2458	**H3p**	H autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors
2459	**H4p**	H autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors
2460	**H5p**	H autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2461	**H6p**	H autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2462	**H7p**	H autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2463	**H8p**	H autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2464	**HTp**	H total index / weighted by polarizability	GETAWAY descriptors
2465	**HATS0p**	leverage-weighted autocorrelation of lag 0 / weighted by polarizability	GETAWAY descriptors
2466	**HATS1p**	leverage-weighted autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors
2467	**HATS2p**	leverage-weighted autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2468	**HATS3p**	leverage-weighted autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors
2469	**HATS4p**	leverage-weighted autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors
2470	**HATS5p**	leverage-weighted autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2471	**HATS6p**	leverage-weighted autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2472	**HATS7p**	leverage-weighted autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2473	**HATS8p**	leverage-weighted autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2474	**HATSp**	leverage-weighted total index / weighted by polarizability	GETAWAY descriptors
2475	**H0i**	H autocorrelation of lag 0 / weighted by ionization potential	GETAWAY descriptors

No.	Name	Description	Block
2476	**H1i**	H autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2477	**H2i**	H autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2478	**H3i**	H autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2479	**H4i**	H autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2480	**H5i**	H autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2481	**H6i**	H autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2482	**H7i**	H autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2483	**H8i**	H autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2484	**HTi**	H total index / weighted by ionization potential	GETAWAY descriptors
2485	**HATS0i**	leverage-weighted autocorrelation of lag 0 / weighted by ionization potential	GETAWAY descriptors
2486	**HATS1i**	leverage-weighted autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2487	**HATS2i**	leverage-weighted autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2488	**HATS3i**	leverage-weighted autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2489	**HATS4i**	leverage-weighted autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2490	**HATS5i**	leverage-weighted autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2491	**HATS6i**	leverage-weighted autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2492	**HATS7i**	leverage-weighted autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2493	**HATS8i**	leverage-weighted autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2494	**HATSi**	leverage-weighted total index / weighted by ionization potential	GETAWAY descriptors

No.	Name	Description	Block
2495	**H0s**	H autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors
2496	**H1s**	H autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2497	**H2s**	H autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2498	**H3s**	H autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2499	**H4s**	H autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2500	**H5s**	H autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2501	**H6s**	H autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2502	**H7s**	H autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2503	**H8s**	H autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2504	**HTs**	H total index / weighted by I-state	GETAWAY descriptors
2505	**HATS0s**	leverage-weighted autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors
2506	**HATS1s**	leverage-weighted autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2507	**HATS2s**	leverage-weighted autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2508	**HATS3s**	leverage-weighted autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2509	**HATS4s**	leverage-weighted autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2510	**HATS5s**	leverage-weighted autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2511	**HATS6s**	leverage-weighted autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2512	**HATS7s**	leverage-weighted autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2513	**HATS8s**	leverage-weighted autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors

No.	Name	Description	Block
2514	**HATSs**	leverage-weighted total index / weighted by I-state	GETAWAY descriptors
2515	**RCON**	Randic-type R matrix connectivity	GETAWAY descriptors
2516	**RARS**	R matrix average row sum	GETAWAY descriptors
2517	**REIG**	first eigenvalue of the R matrix	GETAWAY descriptors
2518	**R1u**	R autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2519	**R2u**	R autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2520	**R3u**	R autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2521	**R4u**	R autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2522	**R5u**	R autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2523	**R6u**	R autocorrelation of lag 6 / unweighted	GETAWAY descriptors
2524	**R7u**	R autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2525	**R8u**	R autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2526	**RTu**	R total index / unweighted	GETAWAY descriptors
2527	**R1u+**	R maximal autocorrelation of lag 1 / unweighted	GETAWAY descriptors
2528	**R2u+**	R maximal autocorrelation of lag 2 / unweighted	GETAWAY descriptors
2529	**R3u+**	R maximal autocorrelation of lag 3 / unweighted	GETAWAY descriptors
2530	**R4u+**	R maximal autocorrelation of lag 4 / unweighted	GETAWAY descriptors
2531	**R5u+**	R maximal autocorrelation of lag 5 / unweighted	GETAWAY descriptors
2532	**R6u+**	R maximal autocorrelation of lag 6 / unweighted	GETAWAY descriptors

No.	Name	Description	Block
2533	**R7u+**	R maximal autocorrelation of lag 7 / unweighted	GETAWAY descriptors
2534	**R8u+**	R maximal autocorrelation of lag 8 / unweighted	GETAWAY descriptors
2535	**RTu+**	R maximal index / unweighted	GETAWAY descriptors
2536	**R1m**	R autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2537	**R2m**	R autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2538	**R3m**	R autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2539	**R4m**	R autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors
2540	**R5m**	R autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2541	**R6m**	R autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2542	**R7m**	R autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors
2543	**R8m**	R autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2544	**RTm**	R total index / weighted by mass	GETAWAY descriptors
2545	**R1m+**	R maximal autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors
2546	**R2m+**	R maximal autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors
2547	**R3m+**	R maximal autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors
2548	**R4m+**	R maximal autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors
2549	**R5m+**	R maximal autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors
2550	**R6m+**	R maximal autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors
2551	**R7m+**	R maximal autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors

No.	Name	Description	Block
2552	**R8m+**	R maximal autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors
2553	**RTm+**	R maximal index / weighted by mass	GETAWAY descriptors
2554	**R1v**	R autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2555	**R2v**	R autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2556	**R3v**	R autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors
2557	**R4v**	R autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2558	**R5v**	R autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2559	**R6v**	R autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2560	**R7v**	R autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2561	**R8v**	R autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors
2562	**RTv**	R total index / weighted by van der Waals volume	GETAWAY descriptors
2563	**R1v+**	R maximal autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors
2564	**R2v+**	R maximal autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors
2565	**R3v+**	R maximal autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors
2566	**R4v+**	R maximal autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors
2567	**R5v+**	R maximal autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors
2568	**R6v+**	R maximal autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors
2569	**R7v+**	R maximal autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors
2570	**R8v+**	R maximal autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors

No.	Name	Description	Block
2571	**RTv+**	R maximal index / weighted by van der Waals volume	GETAWAY descriptors
2572	**R1e**	R autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2573	**R2e**	R autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors
2574	**R3e**	R autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors
2575	**R4e**	R autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors
2576	**R5e**	R autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2577	**R6e**	R autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2578	**R7e**	R autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2579	**R8e**	R autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2580	**RTe**	R total index / weighted by Sanderson electronegativity	GETAWAY descriptors
2581	**R1e+**	R maximal autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2582	**R2e+**	R maximal autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors
2583	**R3e+**	R maximal autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors
2584	**R4e+**	R maximal autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors
2585	**R5e+**	R maximal autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2586	**R6e+**	R maximal autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2587	**R7e+**	R maximal autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2588	**R8e+**	R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2589	**RTe+**	R maximal index / weighted by Sanderson electronegativity	GETAWAY descriptors

No.	Name	Description	Block
2590	**R1p**	R autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors
2591	**R2p**	R autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2592	**R3p**	R autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors
2593	**R4p**	R autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors
2594	**R5p**	R autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2595	**R6p**	R autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2596	**R7p**	R autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2597	**R8p**	R autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2598	**RTp**	R total index / weighted by polarizability	GETAWAY descriptors
2599	**R1p+**	R maximal autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors
2600	**R2p+**	R maximal autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2601	**R3p+**	R maximal autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors
2602	**R4p+**	R maximal autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors
2603	**R5p+**	R maximal autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2604	**R6p+**	R maximal autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2605	**R7p+**	R maximal autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2606	**R8p+**	R maximal autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2607	**RTp+**	R maximal index / weighted by polarizability	GETAWAY descriptors
2608	**R1i**	R autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors

No.	Name	Description	Block
2609	**R2i**	R autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2610	**R3i**	R autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2611	**R4i**	R autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2612	**R5i**	R autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2613	**R6i**	R autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2614	**R7i**	R autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2615	**R8i**	R autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2616	**RTi**	R total index / weighted by ionization potential	GETAWAY descriptors
2617	**R1i+**	R maximal autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2618	**R2i+**	R maximal autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2619	**R3i+**	R maximal autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2620	**R4i+**	R maximal autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2621	**R5i+**	R maximal autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2622	**R6i+**	R maximal autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2623	**R7i+**	R maximal autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2624	**R8i+**	R maximal autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2625	**RTi+**	R maximal index / weighted by ionization potential	GETAWAY descriptors
2626	**R1s**	R autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2627	**R2s**	R autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors

No.	Name	Description	Block
2628	**R3s**	R autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2629	**R4s**	R autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2630	**R5s**	R autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2631	**R6s**	R autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2632	**R7s**	R autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2633	**R8s**	R autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2634	**RTs**	R total index / weighted by I-state	GETAWAY descriptors
2635	**R1s+**	R maximal autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2636	**R2s+**	R maximal autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2637	**R3s+**	R maximal autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2638	**R4s+**	R maximal autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2639	**R5s+**	R maximal autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2640	**R6s+**	R maximal autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2641	**R7s+**	R maximal autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2642	**R8s+**	R maximal autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2643	**RTs+**	R maximal index / weighted by I-state	GETAWAY descriptors
2644	**DP01**	molecular profile no. 1	Randic molecular profiles
2645	**DP02**	molecular profile no. 2	Randic molecular profiles

No.	Name	Description	Block
2646	**DP03**	molecular profile no. 3	Randic molecular profiles
2647	**DP04**	molecular profile no. 4	Randic molecular profiles
2648	**DP05**	molecular profile no. 5	Randic molecular profiles
2649	**DP06**	molecular profile no. 6	Randic molecular profiles
2650	**DP07**	molecular profile no. 7	Randic molecular profiles
2651	**DP08**	molecular profile no. 8	Randic molecular profiles
2652	**DP09**	molecular profile no. 9	Randic molecular profiles
2653	**DP10**	molecular profile no. 10	Randic molecular profiles
2654	**DP11**	molecular profile no. 11	Randic molecular profiles
2655	**DP12**	molecular profile no. 12	Randic molecular profiles
2656	**DP13**	molecular profile no. 13	Randic molecular profiles
2657	**DP14**	molecular profile no. 14	Randic molecular profiles
2658	**DP15**	molecular profile no. 15	Randic molecular profiles
2659	**DP16**	molecular profile no. 16	Randic molecular profiles

No.	Name	Description	Block
2660	**DP17**	molecular profile no. 17	Randic molecular profiles
2661	**DP18**	molecular profile no. 18	Randic molecular profiles
2662	**DP19**	molecular profile no. 19	Randic molecular profiles
2663	**DP20**	molecular profile no. 20	Randic molecular profiles
2664	**SP01**	shape profile no. 1	Randic molecular profiles
2665	**SP02**	shape profile no. 2	Randic molecular profiles
2666	**SP03**	shape profile no. 3	Randic molecular profiles
2667	**SP04**	shape profile no. 4	Randic molecular profiles
2668	**SP05**	shape profile no. 5	Randic molecular profiles
2669	**SP06**	shape profile no. 6	Randic molecular profiles
2670	**SP07**	shape profile no. 7	Randic molecular profiles
2671	**SP08**	shape profile no. 8	Randic molecular profiles
2672	**SP09**	shape profile no. 9	Randic molecular profiles
2673	**SP10**	shape profile no. 10	Randic molecular profiles

No.	Name	Description	Block
2674	**SP11**	shape profile no. 11	Randic molecular profiles
2675	**SP12**	shape profile no. 12	Randic molecular profiles
2676	**SP13**	shape profile no. 13	Randic molecular profiles
2677	**SP14**	shape profile no. 14	Randic molecular profiles
2678	**SP15**	shape profile no. 15	Randic molecular profiles
2679	**SP16**	shape profile no. 16	Randic molecular profiles
2680	**SP17**	shape profile no. 17	Randic molecular profiles
2681	**SP18**	shape profile no. 18	Randic molecular profiles
2682	**SP19**	shape profile no. 19	Randic molecular profiles
2683	**SP20**	shape profile no. 20	Randic molecular profiles
2684	**SHP2**	average shape profile index of order 2	Randic molecular profiles
2685	**nCp**	number of terminal primary C(sp3)	Functional group counts
2686	**nCs**	number of total secondary C(sp3)	Functional group counts
2687	**nCt**	number of total tertiary C(sp3)	Functional group counts
2688	**nCq**	number of total quaternary C(sp3)	Functional group counts

No.	Name	Description	Block
2689	**nCrs**	number of ring secondary C(sp3)	Functional group counts
2690	**nCrt**	number of ring tertiary C(sp3)	Functional group counts
2691	**nCrq**	number of ring quaternary C(sp3)	Functional group counts
2692	**nCar**	number of aromatic C(sp2)	Functional group counts
2693	**nCbH**	number of unsubstituted benzene C(sp2)	Functional group counts
2694	**nCb-**	number of substituted benzene C(sp2)	Functional group counts
2695	**nCconj**	number of non-aromatic conjugated C(sp2)	Functional group counts
2696	**nR=Cp**	number of terminal primary C(sp2)	Functional group counts
2697	**nR=Cs**	number of aliphatic secondary C(sp2)	Functional group counts
2698	**nR=Ct**	number of aliphatic tertiary C(sp2)	Functional group counts
2699	**n=C=**	number of allenes groups	Functional group counts
2700	**nR#CH/X**	number of terminal C(sp)	Functional group counts
2701	**nR#C-**	number of non-terminal C(sp)	Functional group counts
2702	**nROCN**	number of cyanates (aliphatic)	Functional group counts
2703	**nArOCN**	number of cyanates (aromatic)	Functional group counts
2704	**nRNCO**	number of isocyanates (aliphatic)	Functional group counts
2705	**nArNCO**	number of isocyanates (aromatic)	Functional group counts
2706	**nRSCN**	number of thiocyanates (aliphatic)	Functional group counts
2707	**nArSCN**	number of thiocyanates (aromatic)	Functional group counts

No.	Name	Description	Block
2708	**nRNCS**	number of isothiocyanates (aliphatic)	Functional group counts
2709	**nArNCS**	number of isothiocyanates (aromatic)	Functional group counts
2710	**nRCOOH**	number of carboxylic acids (aliphatic)	Functional group counts
2711	**nArCOOH**	number of carboxylic acids (aromatic)	Functional group counts
2712	**nRCOOR**	number of esters (aliphatic)	Functional group counts
2713	**nArCOOR**	number of esters (aromatic)	Functional group counts
2714	**nRCONH2**	number of primary amides (aliphatic)	Functional group counts
2715	**nArCONH2**	number of primary amides (aromatic)	Functional group counts
2716	**nRCONHR**	number of secondary amides (aliphatic)	Functional group counts
2717	**nArCONHR**	number of secondary amides (aromatic)	Functional group counts
2718	**nRCONR2**	number of tertiary amides (aliphatic)	Functional group counts
2719	**nArCONR2**	number of tertiary amides (aromatic)	Functional group counts
2720	**nROCON**	number of (thio-) carbamates (aliphatic)	Functional group counts
2721	**nArOCON**	number of (thio-) carbamates (aromatic)	Functional group counts
2722	**nRCOX**	number of acyl halogenides (aliphatic)	Functional group counts
2723	**nArCOX**	number of acyl halogenides (aromatic)	Functional group counts
2724	**nRCSOH**	number of thioacids (aliphatic)	Functional group counts
2725	**nArCSOH**	number of thioacids (aromatic)	Functional group counts
2726	**nRCSSH**	number of dithioacids (aliphatic)	Functional group counts

No.	Name	Description	Block
2727	**nArCSSH**	number of dithioacids (aromatic)	Functional group counts
2728	**nRCOSR**	number of thioesters (aliphatic)	Functional group counts
2729	**nArCOSR**	number of thioesters (aromatic)	Functional group counts
2730	**nRCSSR**	number of dithioesters (aliphatic)	Functional group counts
2731	**nArCSSR**	number of dithioesters (aromatic)	Functional group counts
2732	**nRCHO**	number of aldehydes (aliphatic)	Functional group counts
2733	**nArCHO**	number of aldehydes (aromatic)	Functional group counts
2734	**nRCO**	number of ketones (aliphatic)	Functional group counts
2735	**nArCO**	number of ketones (aromatic)	Functional group counts
2736	**nCONN**	number of urea (-thio) derivatives	Functional group counts
2737	**nC=O(O)2**	number of carbonate (-thio) derivatives	Functional group counts
2738	**nN=C-N<**	number of amidine derivatives	Functional group counts
2739	**nC(=N)N2**	number of guanidine derivatives	Functional group counts
2740	**nRC=N**	number of imines (aliphatic)	Functional group counts
2741	**nArC=N**	number of imines (aromatic)	Functional group counts
2742	**nRCNO**	number of oximes (aliphatic)	Functional group counts
2743	**nArCNO**	number of oximes (aromatic)	Functional group counts
2744	**nRNH2**	number of primary amines (aliphatic)	Functional group counts
2745	**nArNH2**	number of primary amines (aromatic)	Functional group counts

No.	Name	Description	Block
2746	**nRNHR**	number of secondary amines (aliphatic)	Functional group counts
2747	**nArNHR**	number of secondary amines (aromatic)	Functional group counts
2748	**nRNR2**	number of tertiary amines (aliphatic)	Functional group counts
2749	**nArNR2**	number of tertiary amines (aromatic)	Functional group counts
2750	**nN-N**	number of N hydrazines	Functional group counts
2751	**nN=N**	number of N azo-derivatives	Functional group counts
2752	**nRCN**	number of nitriles (aliphatic)	Functional group counts
2753	**nArCN**	number of nitriles (aromatic)	Functional group counts
2754	**nN+**	number of positively charged N	Functional group counts
2755	**nNq**	number of quaternary N	Functional group counts
2756	**nRNHO**	number of hydroxylamines (aliphatic)	Functional group counts
2757	**nArNHO**	number of hydroxylamines (aromatic)	Functional group counts
2758	**nRNNOx**	number of N-nitroso groups (aliphatic)	Functional group counts
2759	**nArNNOx**	number of N-nitroso groups (aromatic)	Functional group counts
2760	**nRNO**	number of nitroso groups (aliphatic)	Functional group counts
2761	**nArNO**	number of nitroso groups (aromatic)	Functional group counts
2762	**nRNO2**	number of nitro groups (aliphatic)	Functional group counts
2763	**nArNO2**	number of nitro groups (aromatic)	Functional group counts
2764	**nN(CO)2**	number of imides (-thio)	Functional group counts

No.	Name	Description	Block
2765	**nC=N-N<**	number of hydrazones	Functional group counts
2766	**nROH**	number of hydroxyl groups	Functional group counts
2767	**nArOH**	number of aromatic hydroxyls	Functional group counts
2768	**nOHp**	number of primary alcohols	Functional group counts
2769	**nOHs**	number of secondary alcohols	Functional group counts
2770	**nOHt**	number of tertiary alcohols	Functional group counts
2771	**nROR**	number of ethers (aliphatic)	Functional group counts
2772	**nArOR**	number of ethers (aromatic)	Functional group counts
2773	**nROX**	number of hypohalogenides (aliphatic)	Functional group counts
2774	**nArOX**	number of hypohalogenides (aromatic)	Functional group counts
2775	**nO(C=O)2**	number of anhydrides (-thio)	Functional group counts
2776	**nH2O**	number of water molecules	Functional group counts
2777	**nSH**	number of thiols	Functional group counts
2778	**nC=S**	number of thioketones	Functional group counts
2779	**nRSR**	number of sulfides	Functional group counts
2780	**nRSSR**	number of disulfides	Functional group counts
2781	**nSO**	number of sulfoxides	Functional group counts
2782	**nS(=O)2**	number of sulfones	Functional group counts
2783	**nSOH**	number of sulfenic (thio-) acids	Functional group counts

No.	Name	Description	Block
2784	**nSOOH**	number of sulfinic (thio-/dithio-) acids	Functional group counts
2785	**nSO2OH**	number of sulfonic (thio-/dithio-) acids	Functional group counts
2786	**nSO3OH**	number of sulfuric (thio-/dithio-) acids	Functional group counts
2787	**nSO2**	number of sulfites (thio-/dithio-)	Functional group counts
2788	**nSO3**	number of sulfonates (thio-/dithio-)	Functional group counts
2789	**nSO4**	number of sulfates (thio-/dithio-)	Functional group counts
2790	**nSO2N**	number of sulfonamides (thio-/dithio-)	Functional group counts
2791	**nPO3**	number of phosphites/thiophosphites	Functional group counts
2792	**nPO4**	number of phosphates/thiophosphates	Functional group counts
2793	**nPR3**	number of phosphanes	Functional group counts
2794	**nP(=O)O2R**	number of phosphonates (thio-)	Functional group counts
2795	**nP(=O)R3/nPR5**	number of phosphoranes (thio-)	Functional group counts
2796	**nCH2RX**	number of CH2RX	Functional group counts
2797	**nCHR2X**	number of CHR2X	Functional group counts
2798	**nCR3X**	number of CR3X	Functional group counts
2799	**nR=CHX**	number of R=CHX	Functional group counts
2800	**nR=CRX**	number of R=CRX	Functional group counts
2801	**nR#CX**	number of R#CX	Functional group counts
2802	**nCHRX2**	number of CHRX2	Functional group counts

No.	Name	Description	Block
2803	**nCR2X2**	number of CR2X2	Functional group counts
2804	**nR=CX2**	number of R=CX2	Functional group counts
2805	**nCRX3**	number of CRX3	Functional group counts
2806	**nArX**	number of X on aromatic ring	Functional group counts
2807	**nCXr**	number of X on ring C(sp3)	Functional group counts
2808	**nCXr=**	number of X on ring C(sp2)	Functional group counts
2809	**nCconjX**	number of X on exo-conjugated C	Functional group counts
2810	**nAziridines**	number of Aziridines	Functional group counts
2811	**nOxiranes**	number of Oxiranes	Functional group counts
2812	**nThiranes**	number of Thiranes	Functional group counts
2813	**nAzetidines**	number of Azetidines	Functional group counts
2814	**nOxetanes**	number of Oxetanes	Functional group counts
2815	**nThioethanes**	number of Thioethanes	Functional group counts
2816	**nBeta-Lactams**	number of Beta-Lactams	Functional group counts
2817	**nPyrrolidines**	number of Pyrrolidines	Functional group counts
2818	**nOxolanes**	number of Oxolanes	Functional group counts
2819	**ntH-Thiophenes**	number of tetrahydro-thiophenes	Functional group counts
2820	**nPyrroles**	number of Pyrroles	Functional group counts
2821	**nPyrazoles**	number of Pyrazoles	Functional group counts

No.	Name	Description	Block
2822	**nImidazoles**	number of Imidazoles	Functional group counts
2823	**nFuranes**	number of Furanes	Functional group counts
2824	**nThiophenes**	number of Thiophenes	Functional group counts
2825	**nOxazoles**	number of Oxazoles	Functional group counts
2826	**nIsoxazoles**	number of Isoxazoles	Functional group counts
2827	**nThiazoles**	number of Thiazoles	Functional group counts
2828	**nIsothiazoles**	number of Isothiazoles	Functional group counts
2829	**nTriazoles**	number of Triazoles	Functional group counts
2830	**nPyridines**	number of Pyridines	Functional group counts
2831	**nPyridazines**	number of Pyridazines	Functional group counts
2832	**nPyrimidines**	number of Pyrimidines	Functional group counts
2833	**nPyrazines**	number of Pyrazines	Functional group counts
2834	**n135-Triazines**	number of 1-3-5-Triazines	Functional group counts
2835	**n124-Triazines**	number of 1-2-4-Triazines	Functional group counts
2836	**nHDon**	number of donor atoms for H-bonds (N and O)	Functional group counts
2837	**nHAcc**	number of acceptor atoms for H-bonds (N,O,F)	Functional group counts
2838	**nHBonds**	number of intramolecular H-bonds (with N,O,F)	Functional group counts
2839	**C-001**	CH3R / CH4	Atom-centred fragments
2840	**C-002**	CH2R2	Atom-centred fragments

No.	Name	Description	Block
2841	**C-003**	CHR3	Atom-centred fragments
2842	**C-004**	CR4	Atom-centred fragments
2843	**C-005**	CH3X	Atom-centred fragments
2844	**C-006**	CH2RX	Atom-centred fragments
2845	**C-007**	CH2X2	Atom-centred fragments
2846	**C-008**	CHR2X	Atom-centred fragments
2847	**C-009**	CHRX2	Atom-centred fragments
2848	**C-010**	CHX3	Atom-centred fragments
2849	**C-011**	CR3X	Atom-centred fragments
2850	**C-012**	CR2X2	Atom-centred fragments
2851	**C-013**	CRX3	Atom-centred fragments
2852	**C-014**	CX4	Atom-centred fragments
2853	**C-015**	=CH2	Atom-centred fragments
2854	**C-016**	=CHR	Atom-centred fragments
2855	**C-017**	=CR2	Atom-centred fragments
2856	**C-018**	=CHX	Atom-centred fragments
2857	**C-019**	=CRX	Atom-centred fragments
2858	**C-020**	=CX2	Atom-centred fragments
2859	**C-021**	#CH	Atom-centred fragments

No.	Name	Description	Block
2860	**C-022**	#CR / R=C=R	Atom-centred fragments
2861	**C-023**	#CX	Atom-centred fragments
2862	**C-024**	R--CH--R	Atom-centred fragments
2863	**C-025**	R--CR--R	Atom-centred fragments
2864	**C-026**	R--CX--R	Atom-centred fragments
2865	**C-027**	R--CH--X	Atom-centred fragments
2866	**C-028**	R--CR--X	Atom-centred fragments
2867	**C-029**	R--CX--X	Atom-centred fragments
2868	**C-030**	X--CH--X	Atom-centred fragments
2869	**C-031**	X--CR--X	Atom-centred fragments
2870	**C-032**	X--CX--X	Atom-centred fragments
2871	**C-033**	R--CH..X	Atom-centred fragments
2872	**C-034**	R--CR..X	Atom-centred fragments
2873	**C-035**	R--CX..X	Atom-centred fragments
2874	**C-036**	Al-CH=X	Atom-centred fragments
2875	**C-037**	Ar-CH=X	Atom-centred fragments
2876	**C-038**	Al-C(=X)-Al	Atom-centred fragments
2877	**C-039**	Ar-C(=X)-R	Atom-centred fragments
2878	**C-040**	R-C(=X)-X / R-C#X / X=C=X	Atom-centred fragments

No.	Name	Description	Block
2879	**C-041**	X-C(=X)-X	Atom-centred fragments
2880	**C-042**	X--CH..X	Atom-centred fragments
2881	**C-043**	X--CR..X	Atom-centred fragments
2882	**C-044**	X--CX..X	Atom-centred fragments
2883	**H-046**	H attached to C0(sp3) no X attached to next C	Atom-centred fragments
2884	**H-047**	H attached to C1(sp3)/C0(sp2)	Atom-centred fragments
2885	**H-048**	H attached to C2(sp3)/C1(sp2)/C0(sp)	Atom-centred fragments
2886	**H-049**	H attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)	Atom-centred fragments
2887	**H-050**	H attached to heteroatom	Atom-centred fragments
2888	**H-051**	H attached to alpha-C	Atom-centred fragments
2889	**H-052**	H attached to C0(sp3) with 1X attached to next C	Atom-centred fragments
2890	**H-053**	H attached to C0(sp3) with 2X attached to next C	Atom-centred fragments
2891	**H-054**	H attached to C0(sp3) with 3X attached to next C	Atom-centred fragments
2892	**H-055**	H attached to C0(sp3) with 4X attached to next C	Atom-centred fragments
2893	**O-056**	alcohol	Atom-centred fragments
2894	**O-057**	phenol / enol / carboxyl OH	Atom-centred fragments
2895	**O-058**	=O	Atom-centred fragments
2896	**O-059**	Al-O-Al	Atom-centred fragments
2897	**O-060**	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X	Atom-centred fragments

No.	Name	Description	Block
2898	**O-061**	O--	Atom-centred fragments
2899	**O-062**	O- (negatively charged)	Atom-centred fragments
2900	**O-063**	R-O-O-R	Atom-centred fragments
2901	**Se-064**	Any-Se-Any	Atom-centred fragments
2902	**Se-065**	=Se	Atom-centred fragments
2903	**N-066**	Al-NH2	Atom-centred fragments
2904	**N-067**	Al2-NH	Atom-centred fragments
2905	**N-068**	Al3-N	Atom-centred fragments
2906	**N-069**	Ar-NH2 / X-NH2	Atom-centred fragments
2907	**N-070**	Ar-NH-Al	Atom-centred fragments
2908	**N-071**	Ar-NAl2	Atom-centred fragments
2909	**N-072**	RCO-N< / >N-X=X	Atom-centred fragments
2910	**N-073**	Ar2NH / Ar3N / Ar2N-Al / R..N..R	Atom-centred fragments
2911	**N-074**	R#N / R=N-	Atom-centred fragments
2912	**N-075**	R--N--R / R--N--X	Atom-centred fragments
2913	**N-076**	Ar-NO2 / R--N(--R)--O / RO-NO	Atom-centred fragments
2914	**N-077**	Al-NO2	Atom-centred fragments
2915	**N-078**	Ar-N=X / X-N=X	Atom-centred fragments
2916	**N-079**	N+ (positively charged)	Atom-centred fragments

No.	Name	Description	Block
2917	**F-081**	F attached to C1(sp3)	Atom-centred fragments
2918	**F-082**	F attached to C2(sp3)	Atom-centred fragments
2919	**F-083**	F attached to C3(sp3)	Atom-centred fragments
2920	**F-084**	F attached to C1(sp2)	Atom-centred fragments
2921	**F-085**	F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2922	**Cl-086**	Cl attached to C1(sp3)	Atom-centred fragments
2923	**Cl-087**	Cl attached to C2(sp3)	Atom-centred fragments
2924	**Cl-088**	Cl attached to C3(sp3)	Atom-centred fragments
2925	**Cl-089**	Cl attached to C1(sp2)	Atom-centred fragments
2926	**Cl-090**	Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2927	**Br-091**	Br attached to C1(sp3)	Atom-centred fragments
2928	**Br-092**	Br attached to C2(sp3)	Atom-centred fragments
2929	**Br-093**	Br attached to C3(sp3)	Atom-centred fragments
2930	**Br-094**	Br attached to C1(sp2)	Atom-centred fragments
2931	**Br-095**	Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2932	**I-096**	I attached to C1(sp3)	Atom-centred fragments
2933	**I-097**	I attached to C2(sp3)	Atom-centred fragments
2934	**I-098**	I attached to C3(sp3)	Atom-centred fragments
2935	**I-099**	I attached to C1(sp2)	Atom-centred fragments

No.	Name	Description	Block
2936	**I-100**	I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments
2937	**F-101**	fluoride ion	Atom-centred fragments
2938	**Cl-102**	chloride ion	Atom-centred fragments
2939	**Br-103**	bromide ion	Atom-centred fragments
2940	**I-104**	iodide ion	Atom-centred fragments
2941	**S-106**	R-SH	Atom-centred fragments
2942	**S-107**	R2S / RS-SR	Atom-centred fragments
2943	**S-108**	R=S	Atom-centred fragments
2944	**S-109**	R-SO-R	Atom-centred fragments
2945	**S-110**	R-SO2-R	Atom-centred fragments
2946	**Si-111**	>Si<	Atom-centred fragments
2947	**B-112**	>B- as in boranes	Atom-centred fragments
2948	**P-115**	P ylids	Atom-centred fragments
2949	**P-116**	R3-P=X	Atom-centred fragments
2950	**P-117**	X3-P=X (phosphate)	Atom-centred fragments
2951	**P-118**	PX3 (phosphite)	Atom-centred fragments
2952	**P-119**	PR3 (phosphine)	Atom-centred fragments
2953	**P-120**	C-P(X)2=X (phosphonate)	Atom-centred fragments
2954	**SsCH3**	Sum of sCH3 E-states	Atom-type E-state indices

No.	Name	Description	Block
2955	**SdCH2**	Sum of dCH2 E-states	Atom-type E-state indices
2956	**SssCH2**	Sum of ssCH2 E-states	Atom-type E-state indices
2957	**StCH**	Sum of tCH E-states	Atom-type E-state indices
2958	**SdsCH**	Sum of dsCH E-states	Atom-type E-state indices
2959	**SaaCH**	Sum of aaCH E-states	Atom-type E-state indices
2960	**SsssCH**	Sum of sssCH E-states	Atom-type E-state indices
2961	**SddC**	Sum of ddC E-states	Atom-type E-state indices
2962	**StsC**	Sum of tsC E-states	Atom-type E-state indices
2963	**SdssC**	Sum of dssC E-states	Atom-type E-state indices
2964	**SaasC**	Sum of aasC E-states	Atom-type E-state indices
2965	**SaaaC**	Sum of aaaC E-states	Atom-type E-state indices
2966	**SssssC**	Sum of ssssC E-states	Atom-type E-state indices
2967	**SsNH2**	Sum of sNH2 E-states	Atom-type E-state indices
2968	**SssNH**	Sum of ssNH E-states	Atom-type E-state indices
2969	**SdNH**	Sum of dNH E-states	Atom-type E-state indices
2970	**SsssN**	Sum of sssN E-states	Atom-type E-state indices
2971	**SdsN**	Sum of dsN E-states	Atom-type E-state indices
2972	**SaaN**	Sum of aaN E-states	Atom-type E-state indices
2973	**StN**	Sum of tN E-states	Atom-type E-state indices

No.	Name	Description	Block
2974	**SsNH3+**	Sum of sNH3+ E-states	Atom-type E-state indices
2975	**SssNH2+**	Sum of ssNH2+ E-states	Atom-type E-state indices
2976	**SdNH2+**	Sum of dNH2+ E-states	Atom-type E-state indices
2977	**SsssNH+**	Sum of sssNH+ E-states	Atom-type E-state indices
2978	**SssssN+**	Sum of ssssN+ E-states	Atom-type E-state indices
2979	**SddsN**	Sum of ddsN E-states	Atom-type E-state indices
2980	**SaadN**	Sum of aadN E-states	Atom-type E-state indices
2981	**SaasN**	Sum of aasN E-states	Atom-type E-state indices
2982	**SaaNH**	Sum of aaNH E-states	Atom-type E-state indices
2983	**SsOH**	Sum of sOH E-states	Atom-type E-state indices
2984	**SdO**	Sum of dO E-states	Atom-type E-state indices
2985	**SssO**	Sum of ssO E-states	Atom-type E-state indices
2986	**SaaO**	Sum of aaO E-states	Atom-type E-state indices
2987	**SsPH2**	Sum of sPH2 E-states	Atom-type E-state indices
2988	**SssPH**	Sum of ssPH E-states	Atom-type E-state indices
2989	**SsssP**	Sum of sssP E-states	Atom-type E-state indices
2990	**SdsssP**	Sum of dsssP E-states	Atom-type E-state indices
2991	**SddsP**	Sum of ddsP E-states	Atom-type E-state indices
2992	**SsssssP**	Sum of sssssP E-states	Atom-type E-state indices

No.	Name	Description	Block
2993	**SsSH**	Sum of sSH E-states	Atom-type E-state indices
2994	**SdS**	Sum of dS E-states	Atom-type E-state indices
2995	**SssS**	Sum of ssS E-states	Atom-type E-state indices
2996	**SaaS**	Sum of aaS E-states	Atom-type E-state indices
2997	**SdssS**	Sum of dssS E-states	Atom-type E-state indices
2998	**SddssS**	Sum of ddssS E-states	Atom-type E-state indices
2999	**SssssssS**	Sum of ssssssS E-states	Atom-type E-state indices
3000	**SsF**	Sum of sF E-states	Atom-type E-state indices
3001	**SsCl**	Sum of sCl E-states	Atom-type E-state indices
3002	**SsBr**	Sum of sBr E-states	Atom-type E-state indices
3003	**SsI**	Sum of sI E-states	Atom-type E-state indices
3004	**SsLi**	Sum of sLi E-states	Atom-type E-state indices
3005	**SssBe**	Sum of ssBe E-states	Atom-type E-state indices
3006	**SssssBe-**	Sum of ssssBe- E-states	Atom-type E-state indices
3007	**SsBH2**	Sum of sBH2 E-states	Atom-type E-state indices
3008	**SssBH**	Sum of ssBH E-states	Atom-type E-state indices
3009	**SsssB**	Sum of sssB E-states	Atom-type E-state indices
3010	**SssssB-**	Sum of ssssB- E-states	Atom-type E-state indices
3011	**SsGeH3**	Sum of sGeH3 E-states	Atom-type E-state indices

No.	Name	Description	Block
3012	**SssGeH2**	Sum of ssGeH2 E-states	Atom-type E-state indices
3013	**SsssGeH**	Sum of sssGeH E-states	Atom-type E-state indices
3014	**SssssGe**	Sum of ssssGe E-states	Atom-type E-state indices
3015	**SsAsH2**	Sum of sAsH2 E-states	Atom-type E-state indices
3016	**SssAsH**	Sum of ssAsH E-states	Atom-type E-state indices
3017	**SsssAs**	Sum of sssAs E-states	Atom-type E-state indices
3018	**SssssAs**	Sum of sssssAs E-states	Atom-type E-state indices
3019	**SdsssAs**	Sum of dsssAs E-states	Atom-type E-state indices
3020	**SddsAs**	Sum of ddsAs E-states	Atom-type E-state indices
3021	**SsSeH**	Sum of sSeH E-states	Atom-type E-state indices
3022	**SdSe**	Sum of dSe E-states	Atom-type E-state indices
3023	**SssSe**	Sum of ssSe E-states	Atom-type E-state indices
3024	**SaaSe**	Sum of aaSe E-states	Atom-type E-state indices
3025	**SdssSe**	Sum of dssSe E-states	Atom-type E-state indices
3026	**SssssssSe**	Sum of ssssssSe E-states	Atom-type E-state indices
3027	**SddssSe**	Sum of ddssSe E-states	Atom-type E-state indices
3028	**SsSnH3**	Sum of sSnH3 E-states	Atom-type E-state indices
3029	**SssSnH2**	Sum of ssSnH2 E-states	Atom-type E-state indices
3030	**SsssSnH**	Sum of sssSnH E-states	Atom-type E-state indices

No.	Name	Description	Block
3031	**SssssSn**	Sum of ssssSn E-states	Atom-type E-state indices
3032	**SsPbH3**	Sum of sPbH3 E-states	Atom-type E-state indices
3033	**SssPbH2**	Sum of ssPbH2 E-states	Atom-type E-state indices
3034	**SsssPbH**	Sum of sssPbH E-states	Atom-type E-state indices
3035	**SssssPb**	Sum of ssssPb E-states	Atom-type E-state indices
3036	**SsSiH3**	Sum of sSiH3 E-states	Atom-type E-state indices
3037	**SssSiH2**	Sum of ssSiH2 E-states	Atom-type E-state indices
3038	**SsssSiH**	Sum of sssSiH E-states	Atom-type E-state indices
3039	**SssssSi**	Sum of ssssSi E-states	Atom-type E-state indices
3040	**NsCH3**	Number of atoms of type sCH3	Atom-type E-state indices
3041	**NdCH2**	Number of atoms of type dCH2	Atom-type E-state indices
3042	**NssCH2**	Number of atoms of type ssCH2	Atom-type E-state indices
3043	**NtCH**	Number of atoms of type tCH	Atom-type E-state indices
3044	**NdsCH**	Number of atoms of type dsCH	Atom-type E-state indices
3045	**NaaCH**	Number of atoms of type aaCH	Atom-type E-state indices
3046	**NsssCH**	Number of atoms of type sssCH	Atom-type E-state indices
3047	**NddC**	Number of atoms of type ddC	Atom-type E-state indices
3048	**NtsC**	Number of atoms of type tsC	Atom-type E-state indices
3049	**NdssC**	Number of atoms of type dssC	Atom-type E-state indices

No.	Name	Description	Block
3050	**NaasC**	Number of atoms of type aasC	Atom-type E-state indices
3051	**NaaaC**	Number of atoms of type aaaC	Atom-type E-state indices
3052	**NssssC**	Number of atoms of type ssssC	Atom-type E-state indices
3053	**NsNH2**	Number of atoms of type sNH2	Atom-type E-state indices
3054	**NssNH**	Number of atoms of type ssNH	Atom-type E-state indices
3055	**NdNH**	Number of atoms of type dNH	Atom-type E-state indices
3056	**NsssN**	Number of atoms of type sssN	Atom-type E-state indices
3057	**NdsN**	Number of atoms of type dsN	Atom-type E-state indices
3058	**NaaN**	Number of atoms of type aaN	Atom-type E-state indices
3059	**NtN**	Number of atoms of type tN	Atom-type E-state indices
3060	**NsNH3+**	Number of atoms of type sNH3+	Atom-type E-state indices
3061	**NssNH2+**	Number of atoms of type ssNH2+	Atom-type E-state indices
3062	**NdNH2+**	Number of atoms of type dNH2+	Atom-type E-state indices
3063	**NsssNH+**	Number of atoms of type sssNH+	Atom-type E-state indices
3064	**NssssN+**	Number of atoms of type ssssN+	Atom-type E-state indices
3065	**NddsN**	Number of atoms of type ddsN	Atom-type E-state indices
3066	**NaadN**	Number of atoms of type aadN	Atom-type E-state indices
3067	**NaasN**	Number of atoms of type aasN	Atom-type E-state indices
3068	**NaaNH**	Number of atoms of type aaNH	Atom-type E-state indices

No.	Name	Description	Block
3069	**NsOH**	Number of atoms of type sOH	Atom-type E-state indices
3070	**NdO**	Number of atoms of type dO	Atom-type E-state indices
3071	**NssO**	Number of atoms of type ssO	Atom-type E-state indices
3072	**NaaO**	Number of atoms of type aaO	Atom-type E-state indices
3073	**NsPH2**	Number of atoms of type sPH2	Atom-type E-state indices
3074	**NssPH**	Number of atoms of type ssPH	Atom-type E-state indices
3075	**NsssP**	Number of atoms of type sssP	Atom-type E-state indices
3076	**NdsssP**	Number of atoms of type dsssP	Atom-type E-state indices
3077	**NddsP**	Number of atoms of type ddsP	Atom-type E-state indices
3078	**NssssssP**	Number of atoms of type sssssP	Atom-type E-state indices
3079	**NsSH**	Number of atoms of type sSH	Atom-type E-state indices
3080	**NdS**	Number of atoms of type dS	Atom-type E-state indices
3081	**NssS**	Number of atoms of type ssS	Atom-type E-state indices
3082	**NaaS**	Number of atoms of type aaS	Atom-type E-state indices
3083	**NdssS**	Number of atoms of type dssS	Atom-type E-state indices
3084	**NddssS**	Number of atoms of type ddssS	Atom-type E-state indices
3085	**NsssssssS**	Number of atoms of type ssssssS	Atom-type E-state indices
3086	**NsF**	Number of atoms of type sF	Atom-type E-state indices
3087	**NsCl**	Number of atoms of type sCl	Atom-type E-state indices

No.	Name	Description	Block
3088	**NsBr**	Number of atoms of type sBr	Atom-type E-state indices
3089	**NsI**	Number of atoms of type sI	Atom-type E-state indices
3090	**NsLi**	Number of atoms of type sLi	Atom-type E-state indices
3091	**NssBe**	Number of atoms of type ssBe	Atom-type E-state indices
3092	**NssssBe-**	Number of atoms of type ssssBe-	Atom-type E-state indices
3093	**NsBH2**	Number of atoms of type sBH2	Atom-type E-state indices
3094	**NssBH**	Number of atoms of type ssBH	Atom-type E-state indices
3095	**NsssB**	Number of atoms of type sssB	Atom-type E-state indices
3096	**NssssB-**	Number of atoms of type ssssB-	Atom-type E-state indices
3097	**NsGeH3**	Number of atoms of type sGeH3	Atom-type E-state indices
3098	**NssGeH2**	Number of atoms of type ssGeH2	Atom-type E-state indices
3099	**NsssGeH**	Number of atoms of type sssGeH	Atom-type E-state indices
3100	**NssssGe**	Number of atoms of type ssssGe	Atom-type E-state indices
3101	**NsAsH2**	Number of atoms of type sAsH2	Atom-type E-state indices
3102	**NssAsH**	Number of atoms of type ssAsH	Atom-type E-state indices
3103	**NsssAs**	Number of atoms of type sssAs	Atom-type E-state indices
3104	**NssssAs**	Number of atoms of type ssssAs	Atom-type E-state indices
3105	**NdsssAs**	Number of atoms of type dsssAs	Atom-type E-state indices
3106	**NddsAs**	Number of atoms of type ddsAs	Atom-type E-state indices

No.	Name	Description	Block
3107	**NsSeH**	Number of atoms of type sSeH	Atom-type E-state indices
3108	**NdSe**	Number of atoms of type dSe	Atom-type E-state indices
3109	**NssSe**	Number of atoms of type ssSe	Atom-type E-state indices
3110	**NaaSe**	Number of atoms of type aaSe	Atom-type E-state indices
3111	**NdssSe**	Number of atoms of type dssSe	Atom-type E-state indices
3112	**NssssssSe**	Number of atoms of type ssssssSe	Atom-type E-state indices
3113	**NddssSe**	Number of atoms of type ddssSe	Atom-type E-state indices
3114	**NsSnH3**	Number of atoms of type sSnH3	Atom-type E-state indices
3115	**NssSnH2**	Number of atoms of type ssSnH2	Atom-type E-state indices
3116	**NsssSnH**	Number of atoms of type sssSnH	Atom-type E-state indices
3117	**NssssSn**	Number of atoms of type ssssSn	Atom-type E-state indices
3118	**NsPbH3**	Number of atoms of type sPbH3	Atom-type E-state indices
3119	**NssPbH2**	Number of atoms of type ssPbH2	Atom-type E-state indices
3120	**NsssPbH**	Number of atoms of type sssPbH	Atom-type E-state indices
3121	**NssssPb**	Number of atoms of type ssssPb	Atom-type E-state indices
3122	**NsSiH3**	Number of atoms of type sSiH3	Atom-type E-state indices
3123	**NssSiH2**	Number of atoms of type ssSiH2	Atom-type E-state indices
3124	**NsssSiH**	Number of atoms of type sssSiH	Atom-type E-state indices
3125	**NssssSi**	Number of atoms of type ssssSi	Atom-type E-state indices
3126	**CATS2D_00_DD**	CATS2D Donor-Donor at lag 00	CATS 2D

No.	Name	Description	Block
3127	**CATS2D_01_DD**	CATS2D Donor-Donor at lag 01	CATS 2D
3128	**CATS2D_02_DD**	CATS2D Donor-Donor at lag 02	CATS 2D
3129	**CATS2D_03_DD**	CATS2D Donor-Donor at lag 03	CATS 2D
3130	**CATS2D_04_DD**	CATS2D Donor-Donor at lag 04	CATS 2D
3131	**CATS2D_05_DD**	CATS2D Donor-Donor at lag 05	CATS 2D
3132	**CATS2D_06_DD**	CATS2D Donor-Donor at lag 06	CATS 2D
3133	**CATS2D_07_DD**	CATS2D Donor-Donor at lag 07	CATS 2D
3134	**CATS2D_08_DD**	CATS2D Donor-Donor at lag 08	CATS 2D
3135	**CATS2D_09_DD**	CATS2D Donor-Donor at lag 09	CATS 2D
3136	**CATS2D_00_DA**	CATS2D Donor-Acceptor at lag 00	CATS 2D
3137	**CATS2D_01_DA**	CATS2D Donor-Acceptor at lag 01	CATS 2D
3138	**CATS2D_02_DA**	CATS2D Donor-Acceptor at lag 02	CATS 2D
3139	**CATS2D_03_DA**	CATS2D Donor-Acceptor at lag 03	CATS 2D
3140	**CATS2D_04_DA**	CATS2D Donor-Acceptor at lag 04	CATS 2D
3141	**CATS2D_05_DA**	CATS2D Donor-Acceptor at lag 05	CATS 2D
3142	**CATS2D_06_DA**	CATS2D Donor-Acceptor at lag 06	CATS 2D
3143	**CATS2D_07_DA**	CATS2D Donor-Acceptor at lag 07	CATS 2D
3144	**CATS2D_08_DA**	CATS2D Donor-Acceptor at lag 08	CATS 2D
3145	**CATS2D_09_DA**	CATS2D Donor-Acceptor at lag 09	CATS 2D
3146	**CATS2D_00_DP**	CATS2D Donor-Positive at lag 00	CATS 2D
3147	**CATS2D_01_DP**	CATS2D Donor-Positive at lag 01	CATS 2D
3148	**CATS2D_02_DP**	CATS2D Donor-Positive at lag 02	CATS 2D
3149	**CATS2D_03_DP**	CATS2D Donor-Positive at lag 03	CATS 2D
3150	**CATS2D_04_DP**	CATS2D Donor-Positive at lag 04	CATS 2D
3151	**CATS2D_05_DP**	CATS2D Donor-Positive at lag 05	CATS 2D
3152	**CATS2D_06_DP**	CATS2D Donor-Positive at lag 06	CATS 2D
3153	**CATS2D_07_DP**	CATS2D Donor-Positive at lag 07	CATS 2D
3154	**CATS2D_08_DP**	CATS2D Donor-Positive at lag 08	CATS 2D
3155	**CATS2D_09_DP**	CATS2D Donor-Positive at lag 09	CATS 2D
3156	**CATS2D_00_DN**	CATS2D Donor-Negative at lag 00	CATS 2D
3157	**CATS2D_01_DN**	CATS2D Donor-Negative at lag 01	CATS 2D
3158	**CATS2D_02_DN**	CATS2D Donor-Negative at lag 02	CATS 2D

No.	Name	Description	Block
3159	**CATS2D_03_DN**	CATS2D Donor-Negative at lag 03	CATS 2D
3160	**CATS2D_04_DN**	CATS2D Donor-Negative at lag 04	CATS 2D
3161	**CATS2D_05_DN**	CATS2D Donor-Negative at lag 05	CATS 2D
3162	**CATS2D_06_DN**	CATS2D Donor-Negative at lag 06	CATS 2D
3163	**CATS2D_07_DN**	CATS2D Donor-Negative at lag 07	CATS 2D
3164	**CATS2D_08_DN**	CATS2D Donor-Negative at lag 08	CATS 2D
3165	**CATS2D_09_DN**	CATS2D Donor-Negative at lag 09	CATS 2D
3166	**CATS2D_00_DL**	CATS2D Donor-Lipophilic at lag 00	CATS 2D
3167	**CATS2D_01_DL**	CATS2D Donor-Lipophilic at lag 01	CATS 2D
3168	**CATS2D_02_DL**	CATS2D Donor-Lipophilic at lag 02	CATS 2D
3169	**CATS2D_03_DL**	CATS2D Donor-Lipophilic at lag 03	CATS 2D
3170	**CATS2D_04_DL**	CATS2D Donor-Lipophilic at lag 04	CATS 2D
3171	**CATS2D_05_DL**	CATS2D Donor-Lipophilic at lag 05	CATS 2D
3172	**CATS2D_06_DL**	CATS2D Donor-Lipophilic at lag 06	CATS 2D
3173	**CATS2D_07_DL**	CATS2D Donor-Lipophilic at lag 07	CATS 2D
3174	**CATS2D_08_DL**	CATS2D Donor-Lipophilic at lag 08	CATS 2D
3175	**CATS2D_09_DL**	CATS2D Donor-Lipophilic at lag 09	CATS 2D
3176	**CATS2D_00_AA**	CATS2D Acceptor-Acceptor at lag 00	CATS 2D
3177	**CATS2D_01_AA**	CATS2D Acceptor-Acceptor at lag 01	CATS 2D
3178	**CATS2D_02_AA**	CATS2D Acceptor-Acceptor at lag 02	CATS 2D
3179	**CATS2D_03_AA**	CATS2D Acceptor-Acceptor at lag 03	CATS 2D
3180	**CATS2D_04_AA**	CATS2D Acceptor-Acceptor at lag 04	CATS 2D
3181	**CATS2D_05_AA**	CATS2D Acceptor-Acceptor at lag 05	CATS 2D
3182	**CATS2D_06_AA**	CATS2D Acceptor-Acceptor at lag 06	CATS 2D
3183	**CATS2D_07_AA**	CATS2D Acceptor-Acceptor at lag 07	CATS 2D
3184	**CATS2D_08_AA**	CATS2D Acceptor-Acceptor at lag 08	CATS 2D
3185	**CATS2D_09_AA**	CATS2D Acceptor-Acceptor at lag 09	CATS 2D
3186	**CATS2D_00_AP**	CATS2D Acceptor-Positive at lag 00	CATS 2D
3187	**CATS2D_01_AP**	CATS2D Acceptor-Positive at lag 01	CATS 2D
3188	**CATS2D_02_AP**	CATS2D Acceptor-Positive at lag 02	CATS 2D
3189	**CATS2D_03_AP**	CATS2D Acceptor-Positive at lag 03	CATS 2D
3190	**CATS2D_04_AP**	CATS2D Acceptor-Positive at lag 04	CATS 2D

No.	Name	Description	Block
3191	**CATS2D_05_AP**	CATS2D Acceptor-Positive at lag 05	CATS 2D
3192	**CATS2D_06_AP**	CATS2D Acceptor-Positive at lag 06	CATS 2D
3193	**CATS2D_07_AP**	CATS2D Acceptor-Positive at lag 07	CATS 2D
3194	**CATS2D_08_AP**	CATS2D Acceptor-Positive at lag 08	CATS 2D
3195	**CATS2D_09_AP**	CATS2D Acceptor-Positive at lag 09	CATS 2D
3196	**CATS2D_00_AN**	CATS2D Acceptor-Negative at lag 00	CATS 2D
3197	**CATS2D_01_AN**	CATS2D Acceptor-Negative at lag 01	CATS 2D
3198	**CATS2D_02_AN**	CATS2D Acceptor-Negative at lag 02	CATS 2D
3199	**CATS2D_03_AN**	CATS2D Acceptor-Negative at lag 03	CATS 2D
3200	**CATS2D_04_AN**	CATS2D Acceptor-Negative at lag 04	CATS 2D
3201	**CATS2D_05_AN**	CATS2D Acceptor-Negative at lag 05	CATS 2D
3202	**CATS2D_06_AN**	CATS2D Acceptor-Negative at lag 06	CATS 2D
3203	**CATS2D_07_AN**	CATS2D Acceptor-Negative at lag 07	CATS 2D
3204	**CATS2D_08_AN**	CATS2D Acceptor-Negative at lag 08	CATS 2D
3205	**CATS2D_09_AN**	CATS2D Acceptor-Negative at lag 09	CATS 2D
3206	**CATS2D_00_AL**	CATS2D Acceptor-Lipophilic at lag 00	CATS 2D
3207	**CATS2D_01_AL**	CATS2D Acceptor-Lipophilic at lag 01	CATS 2D
3208	**CATS2D_02_AL**	CATS2D Acceptor-Lipophilic at lag 02	CATS 2D
3209	**CATS2D_03_AL**	CATS2D Acceptor-Lipophilic at lag 03	CATS 2D
3210	**CATS2D_04_AL**	CATS2D Acceptor-Lipophilic at lag 04	CATS 2D
3211	**CATS2D_05_AL**	CATS2D Acceptor-Lipophilic at lag 05	CATS 2D
3212	**CATS2D_06_AL**	CATS2D Acceptor-Lipophilic at lag 06	CATS 2D
3213	**CATS2D_07_AL**	CATS2D Acceptor-Lipophilic at lag 07	CATS 2D
3214	**CATS2D_08_AL**	CATS2D Acceptor-Lipophilic at lag 08	CATS 2D
3215	**CATS2D_09_AL**	CATS2D Acceptor-Lipophilic at lag 09	CATS 2D
3216	**CATS2D_00_PP**	CATS2D Positive-Positive at lag 00	CATS 2D
3217	**CATS2D_01_PP**	CATS2D Positive-Positive at lag 01	CATS 2D
3218	**CATS2D_02_PP**	CATS2D Positive-Positive at lag 02	CATS 2D
3219	**CATS2D_03_PP**	CATS2D Positive-Positive at lag 03	CATS 2D
3220	**CATS2D_04_PP**	CATS2D Positive-Positive at lag 04	CATS 2D
3221	**CATS2D_05_PP**	CATS2D Positive-Positive at lag 05	CATS 2D
3222	**CATS2D_06_PP**	CATS2D Positive-Positive at lag 06	CATS 2D

No.	Name	Description	Block
3223	**CATS2D_07_PP**	CATS2D Positive-Positive at lag 07	CATS 2D
3224	**CATS2D_08_PP**	CATS2D Positive-Positive at lag 08	CATS 2D
3225	**CATS2D_09_PP**	CATS2D Positive-Positive at lag 09	CATS 2D
3226	**CATS2D_00_PN**	CATS2D Positive-Negative at lag 00	CATS 2D
3227	**CATS2D_01_PN**	CATS2D Positive-Negative at lag 01	CATS 2D
3228	**CATS2D_02_PN**	CATS2D Positive-Negative at lag 02	CATS 2D
3229	**CATS2D_03_PN**	CATS2D Positive-Negative at lag 03	CATS 2D
3230	**CATS2D_04_PN**	CATS2D Positive-Negative at lag 04	CATS 2D
3231	**CATS2D_05_PN**	CATS2D Positive-Negative at lag 05	CATS 2D
3232	**CATS2D_06_PN**	CATS2D Positive-Negative at lag 06	CATS 2D
3233	**CATS2D_07_PN**	CATS2D Positive-Negative at lag 07	CATS 2D
3234	**CATS2D_08_PN**	CATS2D Positive-Negative at lag 08	CATS 2D
3235	**CATS2D_09_PN**	CATS2D Positive-Negative at lag 09	CATS 2D
3236	**CATS2D_00_PL**	CATS2D Positive-Lipophilic at lag 00	CATS 2D
3237	**CATS2D_01_PL**	CATS2D Positive-Lipophilic at lag 01	CATS 2D
3238	**CATS2D_02_PL**	CATS2D Positive-Lipophilic at lag 02	CATS 2D
3239	**CATS2D_03_PL**	CATS2D Positive-Lipophilic at lag 03	CATS 2D
3240	**CATS2D_04_PL**	CATS2D Positive-Lipophilic at lag 04	CATS 2D
3241	**CATS2D_05_PL**	CATS2D Positive-Lipophilic at lag 05	CATS 2D
3242	**CATS2D_06_PL**	CATS2D Positive-Lipophilic at lag 06	CATS 2D
3243	**CATS2D_07_PL**	CATS2D Positive-Lipophilic at lag 07	CATS 2D
3244	**CATS2D_08_PL**	CATS2D Positive-Lipophilic at lag 08	CATS 2D
3245	**CATS2D_09_PL**	CATS2D Positive-Lipophilic at lag 09	CATS 2D
3246	**CATS2D_00_NN**	CATS2D Negative-Negative at lag 00	CATS 2D
3247	**CATS2D_01_NN**	CATS2D Negative-Negative at lag 01	CATS 2D
3248	**CATS2D_02_NN**	CATS2D Negative-Negative at lag 02	CATS 2D
3249	**CATS2D_03_NN**	CATS2D Negative-Negative at lag 03	CATS 2D
3250	**CATS2D_04_NN**	CATS2D Negative-Negative at lag 04	CATS 2D
3251	**CATS2D_05_NN**	CATS2D Negative-Negative at lag 05	CATS 2D
3252	**CATS2D_06_NN**	CATS2D Negative-Negative at lag 06	CATS 2D
3253	**CATS2D_07_NN**	CATS2D Negative-Negative at lag 07	CATS 2D
3254	**CATS2D_08_NN**	CATS2D Negative-Negative at lag 08	CATS 2D

No.	Name	Description	Block
3255	**CATS2D_09_NN**	CATS2D Negative-Negative at lag 09	CATS 2D
3256	**CATS2D_00_NL**	CATS2D Negative-Lipophilic at lag 00	CATS 2D
3257	**CATS2D_01_NL**	CATS2D Negative-Lipophilic at lag 01	CATS 2D
3258	**CATS2D_02_NL**	CATS2D Negative-Lipophilic at lag 02	CATS 2D
3259	**CATS2D_03_NL**	CATS2D Negative-Lipophilic at lag 03	CATS 2D
3260	**CATS2D_04_NL**	CATS2D Negative-Lipophilic at lag 04	CATS 2D
3261	**CATS2D_05_NL**	CATS2D Negative-Lipophilic at lag 05	CATS 2D
3262	**CATS2D_06_NL**	CATS2D Negative-Lipophilic at lag 06	CATS 2D
3263	**CATS2D_07_NL**	CATS2D Negative-Lipophilic at lag 07	CATS 2D
3264	**CATS2D_08_NL**	CATS2D Negative-Lipophilic at lag 08	CATS 2D
3265	**CATS2D_09_NL**	CATS2D Negative-Lipophilic at lag 09	CATS 2D
3266	**CATS2D_00_LL**	CATS2D Lipophilic-Lipophilic at lag 00	CATS 2D
3267	**CATS2D_01_LL**	CATS2D Lipophilic-Lipophilic at lag 01	CATS 2D
3268	**CATS2D_02_LL**	CATS2D Lipophilic-Lipophilic at lag 02	CATS 2D
3269	**CATS2D_03_LL**	CATS2D Lipophilic-Lipophilic at lag 03	CATS 2D
3270	**CATS2D_04_LL**	CATS2D Lipophilic-Lipophilic at lag 04	CATS 2D
3271	**CATS2D_05_LL**	CATS2D Lipophilic-Lipophilic at lag 05	CATS 2D
3272	**CATS2D_06_LL**	CATS2D Lipophilic-Lipophilic at lag 06	CATS 2D
3273	**CATS2D_07_LL**	CATS2D Lipophilic-Lipophilic at lag 07	CATS 2D
3274	**CATS2D_08_LL**	CATS2D Lipophilic-Lipophilic at lag 08	CATS 2D
3275	**CATS2D_09_LL**	CATS2D Lipophilic-Lipophilic at lag 09	CATS 2D
3276	**T(N..N)**	sum of topological distances between N..N	2D Atom Pairs
3277	**T(N..O)**	sum of topological distances between N..O	2D Atom Pairs
3278	**T(N..S)**	sum of topological distances between N..S	2D Atom Pairs
3279	**T(N..P)**	sum of topological distances between N..P	2D Atom Pairs
3280	**T(N..F)**	sum of topological distances between N..F	2D Atom Pairs
3281	**T(N..Cl)**	sum of topological distances between N..Cl	2D Atom Pairs
3282	**T(N..Br)**	sum of topological distances between N..Br	2D Atom Pairs
3283	**T(N..I)**	sum of topological distances between N..I	2D Atom Pairs
3284	**T(O..O)**	sum of topological distances between O..O	2D Atom Pairs
3285	**T(O..S)**	sum of topological distances between O..S	2D Atom Pairs
3286	**T(O..P)**	sum of topological distances between O..P	2D Atom Pairs

No.	Name	Description	Block
3287	**T(O..F)**	sum of topological distances between O..F	2D Atom Pairs
3288	**T(O..Cl)**	sum of topological distances between O..Cl	2D Atom Pairs
3289	**T(O..Br)**	sum of topological distances between O..Br	2D Atom Pairs
3290	**T(O..I)**	sum of topological distances between O..I	2D Atom Pairs
3291	**T(S..S)**	sum of topological distances between S..S	2D Atom Pairs
3292	**T(S..P)**	sum of topological distances between S..P	2D Atom Pairs
3293	**T(S..F)**	sum of topological distances between S..F	2D Atom Pairs
3294	**T(S..Cl)**	sum of topological distances between S..Cl	2D Atom Pairs
3295	**T(S..Br)**	sum of topological distances between S..Br	2D Atom Pairs
3296	**T(S..I)**	sum of topological distances between S..I	2D Atom Pairs
3297	**T(P..P)**	sum of topological distances between P..P	2D Atom Pairs
3298	**T(P..F)**	sum of topological distances between P..F	2D Atom Pairs
3299	**T(P..Cl)**	sum of topological distances between P..Cl	2D Atom Pairs
3300	**T(P..Br)**	sum of topological distances between P..Br	2D Atom Pairs
3301	**T(P..I)**	sum of topological distances between P..I	2D Atom Pairs
3302	**T(F..F)**	sum of topological distances between F..F	2D Atom Pairs
3303	**T(F..Cl)**	sum of topological distances between F..Cl	2D Atom Pairs
3304	**T(F..Br)**	sum of topological distances between F..Br	2D Atom Pairs
3305	**T(F..I)**	sum of topological distances between F..I	2D Atom Pairs
3306	**T(Cl..Cl)**	sum of topological distances between Cl..Cl	2D Atom Pairs
3307	**T(Cl..Br)**	sum of topological distances between Cl..Br	2D Atom Pairs
3308	**T(Cl..I)**	sum of topological distances between Cl..I	2D Atom Pairs
3309	**T(Br..Br)**	sum of topological distances between Br..Br	2D Atom Pairs
3310	**T(Br..I)**	sum of topological distances between Br..I	2D Atom Pairs
3311	**T(I..I)**	sum of topological distances between I..I	2D Atom Pairs
3312	**B01[C-C]**	Presence/absence of C - C at topological distance 1	2D Atom Pairs
3313	**B01[C-N]**	Presence/absence of C - N at topological distance 1	2D Atom Pairs
3314	**B01[C-O]**	Presence/absence of C - O at topological distance 1	2D Atom Pairs
3315	**B01[C-S]**	Presence/absence of C - S at topological distance 1	2D Atom Pairs
3316	**B01[C-P]**	Presence/absence of C - P at topological distance 1	2D Atom Pairs
3317	**B01[C-F]**	Presence/absence of C - F at topological distance 1	2D Atom Pairs
3318	**B01[C-Cl]**	Presence/absence of C - Cl at topological distance 1	2D Atom Pairs

No.	Name	Description	Block
3319	**B01[C-Br]**	Presence/absence of C - Br at topological distance 1	2D Atom Pairs
3320	**B01[C-I]**	Presence/absence of C - I at topological distance 1	2D Atom Pairs
3321	**B01[C-B]**	Presence/absence of C - B at topological distance 1	2D Atom Pairs
3322	**B01[C-Si]**	Presence/absence of C - Si at topological distance 1	2D Atom Pairs
3323	**B01[C-X]**	Presence/absence of C - X at topological distance 1	2D Atom Pairs
3324	**B01[N-N]**	Presence/absence of N - N at topological distance 1	2D Atom Pairs
3325	**B01[N-O]**	Presence/absence of N - O at topological distance 1	2D Atom Pairs
3326	**B01[N-S]**	Presence/absence of N - S at topological distance 1	2D Atom Pairs
3327	**B01[N-P]**	Presence/absence of N - P at topological distance 1	2D Atom Pairs
3328	**B01[N-F]**	Presence/absence of N - F at topological distance 1	2D Atom Pairs
3329	**B01[N-Cl]**	Presence/absence of N - Cl at topological distance 1	2D Atom Pairs
3330	**B01[N-Br]**	Presence/absence of N - Br at topological distance 1	2D Atom Pairs
3331	**B01[N-I]**	Presence/absence of N - I at topological distance 1	2D Atom Pairs
3332	**B01[N-B]**	Presence/absence of N - B at topological distance 1	2D Atom Pairs
3333	**B01[N-Si]**	Presence/absence of N - Si at topological distance 1	2D Atom Pairs
3334	**B01[N-X]**	Presence/absence of N - X at topological distance 1	2D Atom Pairs
3335	**B01[O-O]**	Presence/absence of O - O at topological distance 1	2D Atom Pairs
3336	**B01[O-S]**	Presence/absence of O - S at topological distance 1	2D Atom Pairs
3337	**B01[O-P]**	Presence/absence of O - P at topological distance 1	2D Atom Pairs
3338	**B01[O-F]**	Presence/absence of O - F at topological distance 1	2D Atom Pairs
3339	**B01[O-Cl]**	Presence/absence of O - Cl at topological distance 1	2D Atom Pairs
3340	**B01[O-Br]**	Presence/absence of O - Br at topological distance 1	2D Atom Pairs
3341	**B01[O-I]**	Presence/absence of O - I at topological distance 1	2D Atom Pairs
3342	**B01[O-B]**	Presence/absence of O - B at topological distance 1	2D Atom Pairs
3343	**B01[O-Si]**	Presence/absence of O - Si at topological distance 1	2D Atom Pairs
3344	**B01[O-X]**	Presence/absence of O - X at topological distance 1	2D Atom Pairs
3345	**B01[S-S]**	Presence/absence of S - S at topological distance 1	2D Atom Pairs
3346	**B01[S-P]**	Presence/absence of S - P at topological distance 1	2D Atom Pairs
3347	**B01[S-F]**	Presence/absence of S - F at topological distance 1	2D Atom Pairs
3348	**B01[S-Cl]**	Presence/absence of S - Cl at topological distance 1	2D Atom Pairs
3349	**B01[S-Br]**	Presence/absence of S - Br at topological distance 1	2D Atom Pairs
3350	**B01[S-I]**	Presence/absence of S - I at topological distance 1	2D Atom Pairs

No.	Name	Description	Block
3351	**B01[S-B]**	Presence/absence of S - B at topological distance 1	2D Atom Pairs
3352	**B01[S-Si]**	Presence/absence of S - Si at topological distance 1	2D Atom Pairs
3353	**B01[S-X]**	Presence/absence of S - X at topological distance 1	2D Atom Pairs
3354	**B01[P-P]**	Presence/absence of P - P at topological distance 1	2D Atom Pairs
3355	**B01[P-F]**	Presence/absence of P - F at topological distance 1	2D Atom Pairs
3356	**B01[P-Cl]**	Presence/absence of P - Cl at topological distance 1	2D Atom Pairs
3357	**B01[P-Br]**	Presence/absence of P - Br at topological distance 1	2D Atom Pairs
3358	**B01[P-I]**	Presence/absence of P - I at topological distance 1	2D Atom Pairs
3359	**B01[P-B]**	Presence/absence of P - B at topological distance 1	2D Atom Pairs
3360	**B01[P-Si]**	Presence/absence of P - Si at topological distance 1	2D Atom Pairs
3361	**B01[P-X]**	Presence/absence of P - X at topological distance 1	2D Atom Pairs
3362	**B01[F-F]**	Presence/absence of F - F at topological distance 1	2D Atom Pairs
3363	**B01[F-Cl]**	Presence/absence of F - Cl at topological distance 1	2D Atom Pairs
3364	**B01[F-Br]**	Presence/absence of F - Br at topological distance 1	2D Atom Pairs
3365	**B01[F-I]**	Presence/absence of F - I at topological distance 1	2D Atom Pairs
3366	**B01[F-B]**	Presence/absence of F - B at topological distance 1	2D Atom Pairs
3367	**B01[F-Si]**	Presence/absence of F - Si at topological distance 1	2D Atom Pairs
3368	**B01[F-X]**	Presence/absence of F - X at topological distance 1	2D Atom Pairs
3369	**B01[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 1	2D Atom Pairs
3370	**B01[Cl-Br]**	Presence/absence of Cl - Br at topological distance 1	2D Atom Pairs
3371	**B01[Cl-I]**	Presence/absence of Cl - I at topological distance 1	2D Atom Pairs
3372	**B01[Cl-B]**	Presence/absence of Cl - B at topological distance 1	2D Atom Pairs
3373	**B01[Cl-Si]**	Presence/absence of Cl - Si at topological distance 1	2D Atom Pairs
3374	**B01[Cl-X]**	Presence/absence of Cl - X at topological distance 1	2D Atom Pairs
3375	**B01[Br-Br]**	Presence/absence of Br - Br at topological distance 1	2D Atom Pairs
3376	**B01[Br-I]**	Presence/absence of Br - I at topological distance 1	2D Atom Pairs
3377	**B01[Br-B]**	Presence/absence of Br - B at topological distance 1	2D Atom Pairs
3378	**B01[Br-Si]**	Presence/absence of Br - Si at topological distance 1	2D Atom Pairs
3379	**B01[Br-X]**	Presence/absence of Br - X at topological distance 1	2D Atom Pairs
3380	**B01[I-I]**	Presence/absence of I - I at topological distance 1	2D Atom Pairs
3381	**B01[I-B]**	Presence/absence of I - B at topological distance 1	2D Atom Pairs
3382	**B01[I-Si]**	Presence/absence of I - Si at topological distance 1	2D Atom Pairs

No.	Name	Description	Block
3383	**B01[I-X]**	Presence/absence of I - X at topological distance 1	2D Atom Pairs
3384	**B01[B-B]**	Presence/absence of B - B at topological distance 1	2D Atom Pairs
3385	**B01[B-Si]**	Presence/absence of B - Si at topological distance 1	2D Atom Pairs
3386	**B01[B-X]**	Presence/absence of B - X at topological distance 1	2D Atom Pairs
3387	**B01[Si-Si]**	Presence/absence of Si - Si at topological distance 1	2D Atom Pairs
3388	**B01[Si-X]**	Presence/absence of Si - X at topological distance 1	2D Atom Pairs
3389	**B01[X-X]**	Presence/absence of X - X at topological distance 1	2D Atom Pairs
3390	**B02[C-C]**	Presence/absence of C - C at topological distance 2	2D Atom Pairs
3391	**B02[C-N]**	Presence/absence of C - N at topological distance 2	2D Atom Pairs
3392	**B02[C-O]**	Presence/absence of C - O at topological distance 2	2D Atom Pairs
3393	**B02[C-S]**	Presence/absence of C - S at topological distance 2	2D Atom Pairs
3394	**B02[C-P]**	Presence/absence of C - P at topological distance 2	2D Atom Pairs
3395	**B02[C-F]**	Presence/absence of C - F at topological distance 2	2D Atom Pairs
3396	**B02[C-Cl]**	Presence/absence of C - Cl at topological distance 2	2D Atom Pairs
3397	**B02[C-Br]**	Presence/absence of C - Br at topological distance 2	2D Atom Pairs
3398	**B02[C-I]**	Presence/absence of C - I at topological distance 2	2D Atom Pairs
3399	**B02[C-B]**	Presence/absence of C - B at topological distance 2	2D Atom Pairs
3400	**B02[C-Si]**	Presence/absence of C - Si at topological distance 2	2D Atom Pairs
3401	**B02[C-X]**	Presence/absence of C - X at topological distance 2	2D Atom Pairs
3402	**B02[N-N]**	Presence/absence of N - N at topological distance 2	2D Atom Pairs
3403	**B02[N-O]**	Presence/absence of N - O at topological distance 2	2D Atom Pairs
3404	**B02[N-S]**	Presence/absence of N - S at topological distance 2	2D Atom Pairs
3405	**B02[N-P]**	Presence/absence of N - P at topological distance 2	2D Atom Pairs
3406	**B02[N-F]**	Presence/absence of N - F at topological distance 2	2D Atom Pairs
3407	**B02[N-Cl]**	Presence/absence of N - Cl at topological distance 2	2D Atom Pairs
3408	**B02[N-Br]**	Presence/absence of N - Br at topological distance 2	2D Atom Pairs
3409	**B02[N-I]**	Presence/absence of N - I at topological distance 2	2D Atom Pairs
3410	**B02[N-B]**	Presence/absence of N - B at topological distance 2	2D Atom Pairs
3411	**B02[N-Si]**	Presence/absence of N - Si at topological distance 2	2D Atom Pairs
3412	**B02[N-X]**	Presence/absence of N - X at topological distance 2	2D Atom Pairs
3413	**B02[O-O]**	Presence/absence of O - O at topological distance 2	2D Atom Pairs
3414	**B02[O-S]**	Presence/absence of O - S at topological distance 2	2D Atom Pairs

No.	Name	Description	Block
3415	**B02[O-P]**	Presence/absence of O - P at topological distance 2	2D Atom Pairs
3416	**B02[O-F]**	Presence/absence of O - F at topological distance 2	2D Atom Pairs
3417	**B02[O-Cl]**	Presence/absence of O - Cl at topological distance 2	2D Atom Pairs
3418	**B02[O-Br]**	Presence/absence of O - Br at topological distance 2	2D Atom Pairs
3419	**B02[O-I]**	Presence/absence of O - I at topological distance 2	2D Atom Pairs
3420	**B02[O-B]**	Presence/absence of O - B at topological distance 2	2D Atom Pairs
3421	**B02[O-Si]**	Presence/absence of O - Si at topological distance 2	2D Atom Pairs
3422	**B02[O-X]**	Presence/absence of O - X at topological distance 2	2D Atom Pairs
3423	**B02[S-S]**	Presence/absence of S - S at topological distance 2	2D Atom Pairs
3424	**B02[S-P]**	Presence/absence of S - P at topological distance 2	2D Atom Pairs
3425	**B02[S-F]**	Presence/absence of S - F at topological distance 2	2D Atom Pairs
3426	**B02[S-Cl]**	Presence/absence of S - Cl at topological distance 2	2D Atom Pairs
3427	**B02[S-Br]**	Presence/absence of S - Br at topological distance 2	2D Atom Pairs
3428	**B02[S-I]**	Presence/absence of S - I at topological distance 2	2D Atom Pairs
3429	**B02[S-B]**	Presence/absence of S - B at topological distance 2	2D Atom Pairs
3430	**B02[S-Si]**	Presence/absence of S - Si at topological distance 2	2D Atom Pairs
3431	**B02[S-X]**	Presence/absence of S - X at topological distance 2	2D Atom Pairs
3432	**B02[P-P]**	Presence/absence of P - P at topological distance 2	2D Atom Pairs
3433	**B02[P-F]**	Presence/absence of P - F at topological distance 2	2D Atom Pairs
3434	**B02[P-Cl]**	Presence/absence of P - Cl at topological distance 2	2D Atom Pairs
3435	**B02[P-Br]**	Presence/absence of P - Br at topological distance 2	2D Atom Pairs
3436	**B02[P-I]**	Presence/absence of P - I at topological distance 2	2D Atom Pairs
3437	**B02[P-B]**	Presence/absence of P - B at topological distance 2	2D Atom Pairs
3438	**B02[P-Si]**	Presence/absence of P - Si at topological distance 2	2D Atom Pairs
3439	**B02[P-X]**	Presence/absence of P - X at topological distance 2	2D Atom Pairs
3440	**B02[F-F]**	Presence/absence of F - F at topological distance 2	2D Atom Pairs
3441	**B02[F-Cl]**	Presence/absence of F - Cl at topological distance 2	2D Atom Pairs
3442	**B02[F-Br]**	Presence/absence of F - Br at topological distance 2	2D Atom Pairs
3443	**B02[F-I]**	Presence/absence of F - I at topological distance 2	2D Atom Pairs
3444	**B02[F-B]**	Presence/absence of F - B at topological distance 2	2D Atom Pairs
3445	**B02[F-Si]**	Presence/absence of F - Si at topological distance 2	2D Atom Pairs
3446	**B02[F-X]**	Presence/absence of F - X at topological distance 2	2D Atom Pairs

No.	Name	Description	Block
3447	**B02[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 2	2D Atom Pairs
3448	**B02[Cl-Br]**	Presence/absence of Cl - Br at topological distance 2	2D Atom Pairs
3449	**B02[Cl-I]**	Presence/absence of Cl - I at topological distance 2	2D Atom Pairs
3450	**B02[Cl-B]**	Presence/absence of Cl - B at topological distance 2	2D Atom Pairs
3451	**B02[Cl-Si]**	Presence/absence of Cl - Si at topological distance 2	2D Atom Pairs
3452	**B02[Cl-X]**	Presence/absence of Cl - X at topological distance 2	2D Atom Pairs
3453	**B02[Br-Br]**	Presence/absence of Br - Br at topological distance 2	2D Atom Pairs
3454	**B02[Br-I]**	Presence/absence of Br - I at topological distance 2	2D Atom Pairs
3455	**B02[Br-B]**	Presence/absence of Br - B at topological distance 2	2D Atom Pairs
3456	**B02[Br-Si]**	Presence/absence of Br - Si at topological distance 2	2D Atom Pairs
3457	**B02[Br-X]**	Presence/absence of Br - X at topological distance 2	2D Atom Pairs
3458	**B02[I-I]**	Presence/absence of I - I at topological distance 2	2D Atom Pairs
3459	**B02[I-B]**	Presence/absence of I - B at topological distance 2	2D Atom Pairs
3460	**B02[I-Si]**	Presence/absence of I - Si at topological distance 2	2D Atom Pairs
3461	**B02[I-X]**	Presence/absence of I - X at topological distance 2	2D Atom Pairs
3462	**B02[B-B]**	Presence/absence of B - B at topological distance 2	2D Atom Pairs
3463	**B02[B-Si]**	Presence/absence of B - Si at topological distance 2	2D Atom Pairs
3464	**B02[B-X]**	Presence/absence of B - X at topological distance 2	2D Atom Pairs
3465	**B02[Si-Si]**	Presence/absence of Si - Si at topological distance 2	2D Atom Pairs
3466	**B02[Si-X]**	Presence/absence of Si - X at topological distance 2	2D Atom Pairs
3467	**B02[X-X]**	Presence/absence of X - X at topological distance 2	2D Atom Pairs
3468	**B03[C-C]**	Presence/absence of C - C at topological distance 3	2D Atom Pairs
3469	**B03[C-N]**	Presence/absence of C - N at topological distance 3	2D Atom Pairs
3470	**B03[C-O]**	Presence/absence of C - O at topological distance 3	2D Atom Pairs
3471	**B03[C-S]**	Presence/absence of C - S at topological distance 3	2D Atom Pairs
3472	**B03[C-P]**	Presence/absence of C - P at topological distance 3	2D Atom Pairs
3473	**B03[C-F]**	Presence/absence of C - F at topological distance 3	2D Atom Pairs
3474	**B03[C-Cl]**	Presence/absence of C - Cl at topological distance 3	2D Atom Pairs
3475	**B03[C-Br]**	Presence/absence of C - Br at topological distance 3	2D Atom Pairs
3476	**B03[C-I]**	Presence/absence of C - I at topological distance 3	2D Atom Pairs
3477	**B03[C-B]**	Presence/absence of C - B at topological distance 3	2D Atom Pairs
3478	**B03[C-Si]**	Presence/absence of C - Si at topological distance 3	2D Atom Pairs

No.	Name	Description	Block
3479	**B03[C-X]**	Presence/absence of C - X at topological distance 3	2D Atom Pairs
3480	**B03[N-N]**	Presence/absence of N - N at topological distance 3	2D Atom Pairs
3481	**B03[N-O]**	Presence/absence of N - O at topological distance 3	2D Atom Pairs
3482	**B03[N-S]**	Presence/absence of N - S at topological distance 3	2D Atom Pairs
3483	**B03[N-P]**	Presence/absence of N - P at topological distance 3	2D Atom Pairs
3484	**B03[N-F]**	Presence/absence of N - F at topological distance 3	2D Atom Pairs
3485	**B03[N-Cl]**	Presence/absence of N - Cl at topological distance 3	2D Atom Pairs
3486	**B03[N-Br]**	Presence/absence of N - Br at topological distance 3	2D Atom Pairs
3487	**B03[N-I]**	Presence/absence of N - I at topological distance 3	2D Atom Pairs
3488	**B03[N-B]**	Presence/absence of N - B at topological distance 3	2D Atom Pairs
3489	**B03[N-Si]**	Presence/absence of N - Si at topological distance 3	2D Atom Pairs
3490	**B03[N-X]**	Presence/absence of N - X at topological distance 3	2D Atom Pairs
3491	**B03[O-O]**	Presence/absence of O - O at topological distance 3	2D Atom Pairs
3492	**B03[O-S]**	Presence/absence of O - S at topological distance 3	2D Atom Pairs
3493	**B03[O-P]**	Presence/absence of O - P at topological distance 3	2D Atom Pairs
3494	**B03[O-F]**	Presence/absence of O - F at topological distance 3	2D Atom Pairs
3495	**B03[O-Cl]**	Presence/absence of O - Cl at topological distance 3	2D Atom Pairs
3496	**B03[O-Br]**	Presence/absence of O - Br at topological distance 3	2D Atom Pairs
3497	**B03[O-I]**	Presence/absence of O - I at topological distance 3	2D Atom Pairs
3498	**B03[O-B]**	Presence/absence of O - B at topological distance 3	2D Atom Pairs
3499	**B03[O-Si]**	Presence/absence of O - Si at topological distance 3	2D Atom Pairs
3500	**B03[O-X]**	Presence/absence of O - X at topological distance 3	2D Atom Pairs
3501	**B03[S-S]**	Presence/absence of S - S at topological distance 3	2D Atom Pairs
3502	**B03[S-P]**	Presence/absence of S - P at topological distance 3	2D Atom Pairs
3503	**B03[S-F]**	Presence/absence of S - F at topological distance 3	2D Atom Pairs
3504	**B03[S-Cl]**	Presence/absence of S - Cl at topological distance 3	2D Atom Pairs
3505	**B03[S-Br]**	Presence/absence of S - Br at topological distance 3	2D Atom Pairs
3506	**B03[S-I]**	Presence/absence of S - I at topological distance 3	2D Atom Pairs
3507	**B03[S-B]**	Presence/absence of S - B at topological distance 3	2D Atom Pairs
3508	**B03[S-Si]**	Presence/absence of S - Si at topological distance 3	2D Atom Pairs
3509	**B03[S-X]**	Presence/absence of S - X at topological distance 3	2D Atom Pairs
3510	**B03[P-P]**	Presence/absence of P - P at topological distance 3	2D Atom Pairs

No.	Name	Description	Block
3511	**B03[P-F]**	Presence/absence of P - F at topological distance 3	2D Atom Pairs
3512	**B03[P-Cl]**	Presence/absence of P - Cl at topological distance 3	2D Atom Pairs
3513	**B03[P-Br]**	Presence/absence of P - Br at topological distance 3	2D Atom Pairs
3514	**B03[P-I]**	Presence/absence of P - I at topological distance 3	2D Atom Pairs
3515	**B03[P-B]**	Presence/absence of P - B at topological distance 3	2D Atom Pairs
3516	**B03[P-Si]**	Presence/absence of P - Si at topological distance 3	2D Atom Pairs
3517	**B03[P-X]**	Presence/absence of P - X at topological distance 3	2D Atom Pairs
3518	**B03[F-F]**	Presence/absence of F - F at topological distance 3	2D Atom Pairs
3519	**B03[F-Cl]**	Presence/absence of F - Cl at topological distance 3	2D Atom Pairs
3520	**B03[F-Br]**	Presence/absence of F - Br at topological distance 3	2D Atom Pairs
3521	**B03[F-I]**	Presence/absence of F - I at topological distance 3	2D Atom Pairs
3522	**B03[F-B]**	Presence/absence of F - B at topological distance 3	2D Atom Pairs
3523	**B03[F-Si]**	Presence/absence of F - Si at topological distance 3	2D Atom Pairs
3524	**B03[F-X]**	Presence/absence of F - X at topological distance 3	2D Atom Pairs
3525	**B03[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 3	2D Atom Pairs
3526	**B03[Cl-Br]**	Presence/absence of Cl - Br at topological distance 3	2D Atom Pairs
3527	**B03[Cl-I]**	Presence/absence of Cl - I at topological distance 3	2D Atom Pairs
3528	**B03[Cl-B]**	Presence/absence of Cl - B at topological distance 3	2D Atom Pairs
3529	**B03[Cl-Si]**	Presence/absence of Cl - Si at topological distance 3	2D Atom Pairs
3530	**B03[Cl-X]**	Presence/absence of Cl - X at topological distance 3	2D Atom Pairs
3531	**B03[Br-Br]**	Presence/absence of Br - Br at topological distance 3	2D Atom Pairs
3532	**B03[Br-I]**	Presence/absence of Br - I at topological distance 3	2D Atom Pairs
3533	**B03[Br-B]**	Presence/absence of Br - B at topological distance 3	2D Atom Pairs
3534	**B03[Br-Si]**	Presence/absence of Br - Si at topological distance 3	2D Atom Pairs
3535	**B03[Br-X]**	Presence/absence of Br - X at topological distance 3	2D Atom Pairs
3536	**B03[I-I]**	Presence/absence of I - I at topological distance 3	2D Atom Pairs
3537	**B03[I-B]**	Presence/absence of I - B at topological distance 3	2D Atom Pairs
3538	**B03[I-Si]**	Presence/absence of I - Si at topological distance 3	2D Atom Pairs
3539	**B03[I-X]**	Presence/absence of I - X at topological distance 3	2D Atom Pairs
3540	**B03[B-B]**	Presence/absence of B - B at topological distance 3	2D Atom Pairs
3541	**B03[B-Si]**	Presence/absence of B - Si at topological distance 3	2D Atom Pairs
3542	**B03[B-X]**	Presence/absence of B - X at topological distance 3	2D Atom Pairs

No.	Name	Description	Block
3543	**B03[Si-Si]**	Presence/absence of Si - Si at topological distance 3	2D Atom Pairs
3544	**B03[Si-X]**	Presence/absence of Si - X at topological distance 3	2D Atom Pairs
3545	**B03[X-X]**	Presence/absence of X - X at topological distance 3	2D Atom Pairs
3546	**B04[C-C]**	Presence/absence of C - C at topological distance 4	2D Atom Pairs
3547	**B04[C-N]**	Presence/absence of C - N at topological distance 4	2D Atom Pairs
3548	**B04[C-O]**	Presence/absence of C - O at topological distance 4	2D Atom Pairs
3549	**B04[C-S]**	Presence/absence of C - S at topological distance 4	2D Atom Pairs
3550	**B04[C-P]**	Presence/absence of C - P at topological distance 4	2D Atom Pairs
3551	**B04[C-F]**	Presence/absence of C - F at topological distance 4	2D Atom Pairs
3552	**B04[C-Cl]**	Presence/absence of C - Cl at topological distance 4	2D Atom Pairs
3553	**B04[C-Br]**	Presence/absence of C - Br at topological distance 4	2D Atom Pairs
3554	**B04[C-I]**	Presence/absence of C - I at topological distance 4	2D Atom Pairs
3555	**B04[C-B]**	Presence/absence of C - B at topological distance 4	2D Atom Pairs
3556	**B04[C-Si]**	Presence/absence of C - Si at topological distance 4	2D Atom Pairs
3557	**B04[C-X]**	Presence/absence of C - X at topological distance 4	2D Atom Pairs
3558	**B04[N-N]**	Presence/absence of N - N at topological distance 4	2D Atom Pairs
3559	**B04[N-O]**	Presence/absence of N - O at topological distance 4	2D Atom Pairs
3560	**B04[N-S]**	Presence/absence of N - S at topological distance 4	2D Atom Pairs
3561	**B04[N-P]**	Presence/absence of N - P at topological distance 4	2D Atom Pairs
3562	**B04[N-F]**	Presence/absence of N - F at topological distance 4	2D Atom Pairs
3563	**B04[N-Cl]**	Presence/absence of N - Cl at topological distance 4	2D Atom Pairs
3564	**B04[N-Br]**	Presence/absence of N - Br at topological distance 4	2D Atom Pairs
3565	**B04[N-I]**	Presence/absence of N - I at topological distance 4	2D Atom Pairs
3566	**B04[N-B]**	Presence/absence of N - B at topological distance 4	2D Atom Pairs
3567	**B04[N-Si]**	Presence/absence of N - Si at topological distance 4	2D Atom Pairs
3568	**B04[N-X]**	Presence/absence of N - X at topological distance 4	2D Atom Pairs
3569	**B04[O-O]**	Presence/absence of O - O at topological distance 4	2D Atom Pairs
3570	**B04[O-S]**	Presence/absence of O - S at topological distance 4	2D Atom Pairs
3571	**B04[O-P]**	Presence/absence of O - P at topological distance 4	2D Atom Pairs
3572	**B04[O-F]**	Presence/absence of O - F at topological distance 4	2D Atom Pairs
3573	**B04[O-Cl]**	Presence/absence of O - Cl at topological distance 4	2D Atom Pairs
3574	**B04[O-Br]**	Presence/absence of O - Br at topological distance 4	2D Atom Pairs

No.	Name	Description	Block
3575	**B04[O-I]**	Presence/absence of O - I at topological distance 4	2D Atom Pairs
3576	**B04[O-B]**	Presence/absence of O - B at topological distance 4	2D Atom Pairs
3577	**B04[O-Si]**	Presence/absence of O - Si at topological distance 4	2D Atom Pairs
3578	**B04[O-X]**	Presence/absence of O - X at topological distance 4	2D Atom Pairs
3579	**B04[S-S]**	Presence/absence of S - S at topological distance 4	2D Atom Pairs
3580	**B04[S-P]**	Presence/absence of S - P at topological distance 4	2D Atom Pairs
3581	**B04[S-F]**	Presence/absence of S - F at topological distance 4	2D Atom Pairs
3582	**B04[S-Cl]**	Presence/absence of S - Cl at topological distance 4	2D Atom Pairs
3583	**B04[S-Br]**	Presence/absence of S - Br at topological distance 4	2D Atom Pairs
3584	**B04[S-I]**	Presence/absence of S - I at topological distance 4	2D Atom Pairs
3585	**B04[S-B]**	Presence/absence of S - B at topological distance 4	2D Atom Pairs
3586	**B04[S-Si]**	Presence/absence of S - Si at topological distance 4	2D Atom Pairs
3587	**B04[S-X]**	Presence/absence of S - X at topological distance 4	2D Atom Pairs
3588	**B04[P-P]**	Presence/absence of P - P at topological distance 4	2D Atom Pairs
3589	**B04[P-F]**	Presence/absence of P - F at topological distance 4	2D Atom Pairs
3590	**B04[P-Cl]**	Presence/absence of P - Cl at topological distance 4	2D Atom Pairs
3591	**B04[P-Br]**	Presence/absence of P - Br at topological distance 4	2D Atom Pairs
3592	**B04[P-I]**	Presence/absence of P - I at topological distance 4	2D Atom Pairs
3593	**B04[P-B]**	Presence/absence of P - B at topological distance 4	2D Atom Pairs
3594	**B04[P-Si]**	Presence/absence of P - Si at topological distance 4	2D Atom Pairs
3595	**B04[P-X]**	Presence/absence of P - X at topological distance 4	2D Atom Pairs
3596	**B04[F-F]**	Presence/absence of F - F at topological distance 4	2D Atom Pairs
3597	**B04[F-Cl]**	Presence/absence of F - Cl at topological distance 4	2D Atom Pairs
3598	**B04[F-Br]**	Presence/absence of F - Br at topological distance 4	2D Atom Pairs
3599	**B04[F-I]**	Presence/absence of F - I at topological distance 4	2D Atom Pairs
3600	**B04[F-B]**	Presence/absence of F - B at topological distance 4	2D Atom Pairs
3601	**B04[F-Si]**	Presence/absence of F - Si at topological distance 4	2D Atom Pairs
3602	**B04[F-X]**	Presence/absence of F - X at topological distance 4	2D Atom Pairs
3603	**B04[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 4	2D Atom Pairs
3604	**B04[Cl-Br]**	Presence/absence of Cl - Br at topological distance 4	2D Atom Pairs
3605	**B04[Cl-I]**	Presence/absence of Cl - I at topological distance 4	2D Atom Pairs
3606	**B04[Cl-B]**	Presence/absence of Cl - B at topological distance 4	2D Atom Pairs

No.	Name	Description	Block
3607	**B04[Cl-Si]**	Presence/absence of Cl - Si at topological distance 4	2D Atom Pairs
3608	**B04[Cl-X]**	Presence/absence of Cl - X at topological distance 4	2D Atom Pairs
3609	**B04[Br-Br]**	Presence/absence of Br - Br at topological distance 4	2D Atom Pairs
3610	**B04[Br-I]**	Presence/absence of Br - I at topological distance 4	2D Atom Pairs
3611	**B04[Br-B]**	Presence/absence of Br - B at topological distance 4	2D Atom Pairs
3612	**B04[Br-Si]**	Presence/absence of Br - Si at topological distance 4	2D Atom Pairs
3613	**B04[Br-X]**	Presence/absence of Br - X at topological distance 4	2D Atom Pairs
3614	**B04[I-I]**	Presence/absence of I - I at topological distance 4	2D Atom Pairs
3615	**B04[I-B]**	Presence/absence of I - B at topological distance 4	2D Atom Pairs
3616	**B04[I-Si]**	Presence/absence of I - Si at topological distance 4	2D Atom Pairs
3617	**B04[I-X]**	Presence/absence of I - X at topological distance 4	2D Atom Pairs
3618	**B04[B-B]**	Presence/absence of B - B at topological distance 4	2D Atom Pairs
3619	**B04[B-Si]**	Presence/absence of B - Si at topological distance 4	2D Atom Pairs
3620	**B04[B-X]**	Presence/absence of B - X at topological distance 4	2D Atom Pairs
3621	**B04[Si-Si]**	Presence/absence of Si - Si at topological distance 4	2D Atom Pairs
3622	**B04[Si-X]**	Presence/absence of Si - X at topological distance 4	2D Atom Pairs
3623	**B04[X-X]**	Presence/absence of X - X at topological distance 4	2D Atom Pairs
3624	**B05[C-C]**	Presence/absence of C - C at topological distance 5	2D Atom Pairs
3625	**B05[C-N]**	Presence/absence of C - N at topological distance 5	2D Atom Pairs
3626	**B05[C-O]**	Presence/absence of C - O at topological distance 5	2D Atom Pairs
3627	**B05[C-S]**	Presence/absence of C - S at topological distance 5	2D Atom Pairs
3628	**B05[C-P]**	Presence/absence of C - P at topological distance 5	2D Atom Pairs
3629	**B05[C-F]**	Presence/absence of C - F at topological distance 5	2D Atom Pairs
3630	**B05[C-Cl]**	Presence/absence of C - Cl at topological distance 5	2D Atom Pairs
3631	**B05[C-Br]**	Presence/absence of C - Br at topological distance 5	2D Atom Pairs
3632	**B05[C-I]**	Presence/absence of C - I at topological distance 5	2D Atom Pairs
3633	**B05[C-B]**	Presence/absence of C - B at topological distance 5	2D Atom Pairs
3634	**B05[C-Si]**	Presence/absence of C - Si at topological distance 5	2D Atom Pairs
3635	**B05[C-X]**	Presence/absence of C - X at topological distance 5	2D Atom Pairs
3636	**B05[N-N]**	Presence/absence of N - N at topological distance 5	2D Atom Pairs
3637	**B05[N-O]**	Presence/absence of N - O at topological distance 5	2D Atom Pairs
3638	**B05[N-S]**	Presence/absence of N - S at topological distance 5	2D Atom Pairs

No.	Name	Description	Block
3639	**B05[N-P]**	Presence/absence of N - P at topological distance 5	2D Atom Pairs
3640	**B05[N-F]**	Presence/absence of N - F at topological distance 5	2D Atom Pairs
3641	**B05[N-Cl]**	Presence/absence of N - Cl at topological distance 5	2D Atom Pairs
3642	**B05[N-Br]**	Presence/absence of N - Br at topological distance 5	2D Atom Pairs
3643	**B05[N-I]**	Presence/absence of N - I at topological distance 5	2D Atom Pairs
3644	**B05[N-B]**	Presence/absence of N - B at topological distance 5	2D Atom Pairs
3645	**B05[N-Si]**	Presence/absence of N - Si at topological distance 5	2D Atom Pairs
3646	**B05[N-X]**	Presence/absence of N - X at topological distance 5	2D Atom Pairs
3647	**B05[O-O]**	Presence/absence of O - O at topological distance 5	2D Atom Pairs
3648	**B05[O-S]**	Presence/absence of O - S at topological distance 5	2D Atom Pairs
3649	**B05[O-P]**	Presence/absence of O - P at topological distance 5	2D Atom Pairs
3650	**B05[O-F]**	Presence/absence of O - F at topological distance 5	2D Atom Pairs
3651	**B05[O-Cl]**	Presence/absence of O - Cl at topological distance 5	2D Atom Pairs
3652	**B05[O-Br]**	Presence/absence of O - Br at topological distance 5	2D Atom Pairs
3653	**B05[O-I]**	Presence/absence of O - I at topological distance 5	2D Atom Pairs
3654	**B05[O-B]**	Presence/absence of O - B at topological distance 5	2D Atom Pairs
3655	**B05[O-Si]**	Presence/absence of O - Si at topological distance 5	2D Atom Pairs
3656	**B05[O-X]**	Presence/absence of O - X at topological distance 5	2D Atom Pairs
3657	**B05[S-S]**	Presence/absence of S - S at topological distance 5	2D Atom Pairs
3658	**B05[S-P]**	Presence/absence of S - P at topological distance 5	2D Atom Pairs
3659	**B05[S-F]**	Presence/absence of S - F at topological distance 5	2D Atom Pairs
3660	**B05[S-Cl]**	Presence/absence of S - Cl at topological distance 5	2D Atom Pairs
3661	**B05[S-Br]**	Presence/absence of S - Br at topological distance 5	2D Atom Pairs
3662	**B05[S-I]**	Presence/absence of S - I at topological distance 5	2D Atom Pairs
3663	**B05[S-B]**	Presence/absence of S - B at topological distance 5	2D Atom Pairs
3664	**B05[S-Si]**	Presence/absence of S - Si at topological distance 5	2D Atom Pairs
3665	**B05[S-X]**	Presence/absence of S - X at topological distance 5	2D Atom Pairs
3666	**B05[P-P]**	Presence/absence of P - P at topological distance 5	2D Atom Pairs
3667	**B05[P-F]**	Presence/absence of P - F at topological distance 5	2D Atom Pairs
3668	**B05[P-Cl]**	Presence/absence of P - Cl at topological distance 5	2D Atom Pairs
3669	**B05[P-Br]**	Presence/absence of P - Br at topological distance 5	2D Atom Pairs
3670	**B05[P-I]**	Presence/absence of P - I at topological distance 5	2D Atom Pairs

No.	Name	Description	Block
3671	**B05[P-B]**	Presence/absence of P - B at topological distance 5	2D Atom Pairs
3672	**B05[P-Si]**	Presence/absence of P - Si at topological distance 5	2D Atom Pairs
3673	**B05[P-X]**	Presence/absence of P - X at topological distance 5	2D Atom Pairs
3674	**B05[F-F]**	Presence/absence of F - F at topological distance 5	2D Atom Pairs
3675	**B05[F-Cl]**	Presence/absence of F - Cl at topological distance 5	2D Atom Pairs
3676	**B05[F-Br]**	Presence/absence of F - Br at topological distance 5	2D Atom Pairs
3677	**B05[F-I]**	Presence/absence of F - I at topological distance 5	2D Atom Pairs
3678	**B05[F-B]**	Presence/absence of F - B at topological distance 5	2D Atom Pairs
3679	**B05[F-Si]**	Presence/absence of F - Si at topological distance 5	2D Atom Pairs
3680	**B05[F-X]**	Presence/absence of F - X at topological distance 5	2D Atom Pairs
3681	**B05[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 5	2D Atom Pairs
3682	**B05[Cl-Br]**	Presence/absence of Cl - Br at topological distance 5	2D Atom Pairs
3683	**B05[Cl-I]**	Presence/absence of Cl - I at topological distance 5	2D Atom Pairs
3684	**B05[Cl-B]**	Presence/absence of Cl - B at topological distance 5	2D Atom Pairs
3685	**B05[Cl-Si]**	Presence/absence of Cl - Si at topological distance 5	2D Atom Pairs
3686	**B05[Cl-X]**	Presence/absence of Cl - X at topological distance 5	2D Atom Pairs
3687	**B05[Br-Br]**	Presence/absence of Br - Br at topological distance 5	2D Atom Pairs
3688	**B05[Br-I]**	Presence/absence of Br - I at topological distance 5	2D Atom Pairs
3689	**B05[Br-B]**	Presence/absence of Br - B at topological distance 5	2D Atom Pairs
3690	**B05[Br-Si]**	Presence/absence of Br - Si at topological distance 5	2D Atom Pairs
3691	**B05[Br-X]**	Presence/absence of Br - X at topological distance 5	2D Atom Pairs
3692	**B05[I-I]**	Presence/absence of I - I at topological distance 5	2D Atom Pairs
3693	**B05[I-B]**	Presence/absence of I - B at topological distance 5	2D Atom Pairs
3694	**B05[I-Si]**	Presence/absence of I - Si at topological distance 5	2D Atom Pairs
3695	**B05[I-X]**	Presence/absence of I - X at topological distance 5	2D Atom Pairs
3696	**B05[B-B]**	Presence/absence of B - B at topological distance 5	2D Atom Pairs
3697	**B05[B-Si]**	Presence/absence of B - Si at topological distance 5	2D Atom Pairs
3698	**B05[B-X]**	Presence/absence of B - X at topological distance 5	2D Atom Pairs
3699	**B05[Si-Si]**	Presence/absence of Si - Si at topological distance 5	2D Atom Pairs
3700	**B05[Si-X]**	Presence/absence of Si - X at topological distance 5	2D Atom Pairs
3701	**B05[X-X]**	Presence/absence of X - X at topological distance 5	2D Atom Pairs
3702	**B06[C-C]**	Presence/absence of C - C at topological distance 6	2D Atom Pairs

No.	Name	Description	Block
3703	**B06[C-N]**	Presence/absence of C - N at topological distance 6	2D Atom Pairs
3704	**B06[C-O]**	Presence/absence of C - O at topological distance 6	2D Atom Pairs
3705	**B06[C-S]**	Presence/absence of C - S at topological distance 6	2D Atom Pairs
3706	**B06[C-P]**	Presence/absence of C - P at topological distance 6	2D Atom Pairs
3707	**B06[C-F]**	Presence/absence of C - F at topological distance 6	2D Atom Pairs
3708	**B06[C-Cl]**	Presence/absence of C - Cl at topological distance 6	2D Atom Pairs
3709	**B06[C-Br]**	Presence/absence of C - Br at topological distance 6	2D Atom Pairs
3710	**B06[C-I]**	Presence/absence of C - I at topological distance 6	2D Atom Pairs
3711	**B06[C-B]**	Presence/absence of C - B at topological distance 6	2D Atom Pairs
3712	**B06[C-Si]**	Presence/absence of C - Si at topological distance 6	2D Atom Pairs
3713	**B06[C-X]**	Presence/absence of C - X at topological distance 6	2D Atom Pairs
3714	**B06[N-N]**	Presence/absence of N - N at topological distance 6	2D Atom Pairs
3715	**B06[N-O]**	Presence/absence of N - O at topological distance 6	2D Atom Pairs
3716	**B06[N-S]**	Presence/absence of N - S at topological distance 6	2D Atom Pairs
3717	**B06[N-P]**	Presence/absence of N - P at topological distance 6	2D Atom Pairs
3718	**B06[N-F]**	Presence/absence of N - F at topological distance 6	2D Atom Pairs
3719	**B06[N-Cl]**	Presence/absence of N - Cl at topological distance 6	2D Atom Pairs
3720	**B06[N-Br]**	Presence/absence of N - Br at topological distance 6	2D Atom Pairs
3721	**B06[N-I]**	Presence/absence of N - I at topological distance 6	2D Atom Pairs
3722	**B06[N-B]**	Presence/absence of N - B at topological distance 6	2D Atom Pairs
3723	**B06[N-Si]**	Presence/absence of N - Si at topological distance 6	2D Atom Pairs
3724	**B06[N-X]**	Presence/absence of N - X at topological distance 6	2D Atom Pairs
3725	**B06[O-O]**	Presence/absence of O - O at topological distance 6	2D Atom Pairs
3726	**B06[O-S]**	Presence/absence of O - S at topological distance 6	2D Atom Pairs
3727	**B06[O-P]**	Presence/absence of O - P at topological distance 6	2D Atom Pairs
3728	**B06[O-F]**	Presence/absence of O - F at topological distance 6	2D Atom Pairs
3729	**B06[O-Cl]**	Presence/absence of O - Cl at topological distance 6	2D Atom Pairs
3730	**B06[O-Br]**	Presence/absence of O - Br at topological distance 6	2D Atom Pairs
3731	**B06[O-I]**	Presence/absence of O - I at topological distance 6	2D Atom Pairs
3732	**B06[O-B]**	Presence/absence of O - B at topological distance 6	2D Atom Pairs
3733	**B06[O-Si]**	Presence/absence of O - Si at topological distance 6	2D Atom Pairs
3734	**B06[O-X]**	Presence/absence of O - X at topological distance 6	2D Atom Pairs

No.	Name	Description	Block
3735	**B06[S-S]**	Presence/absence of S - S at topological distance 6	2D Atom Pairs
3736	**B06[S-P]**	Presence/absence of S - P at topological distance 6	2D Atom Pairs
3737	**B06[S-F]**	Presence/absence of S - F at topological distance 6	2D Atom Pairs
3738	**B06[S-Cl]**	Presence/absence of S - Cl at topological distance 6	2D Atom Pairs
3739	**B06[S-Br]**	Presence/absence of S - Br at topological distance 6	2D Atom Pairs
3740	**B06[S-I]**	Presence/absence of S - I at topological distance 6	2D Atom Pairs
3741	**B06[S-B]**	Presence/absence of S - B at topological distance 6	2D Atom Pairs
3742	**B06[S-Si]**	Presence/absence of S - Si at topological distance 6	2D Atom Pairs
3743	**B06[S-X]**	Presence/absence of S - X at topological distance 6	2D Atom Pairs
3744	**B06[P-P]**	Presence/absence of P - P at topological distance 6	2D Atom Pairs
3745	**B06[P-F]**	Presence/absence of P - F at topological distance 6	2D Atom Pairs
3746	**B06[P-Cl]**	Presence/absence of P - Cl at topological distance 6	2D Atom Pairs
3747	**B06[P-Br]**	Presence/absence of P - Br at topological distance 6	2D Atom Pairs
3748	**B06[P-I]**	Presence/absence of P - I at topological distance 6	2D Atom Pairs
3749	**B06[P-B]**	Presence/absence of P - B at topological distance 6	2D Atom Pairs
3750	**B06[P-Si]**	Presence/absence of P - Si at topological distance 6	2D Atom Pairs
3751	**B06[P-X]**	Presence/absence of P - X at topological distance 6	2D Atom Pairs
3752	**B06[F-F]**	Presence/absence of F - F at topological distance 6	2D Atom Pairs
3753	**B06[F-Cl]**	Presence/absence of F - Cl at topological distance 6	2D Atom Pairs
3754	**B06[F-Br]**	Presence/absence of F - Br at topological distance 6	2D Atom Pairs
3755	**B06[F-I]**	Presence/absence of F - I at topological distance 6	2D Atom Pairs
3756	**B06[F-B]**	Presence/absence of F - B at topological distance 6	2D Atom Pairs
3757	**B06[F-Si]**	Presence/absence of F - Si at topological distance 6	2D Atom Pairs
3758	**B06[F-X]**	Presence/absence of F - X at topological distance 6	2D Atom Pairs
3759	**B06[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 6	2D Atom Pairs
3760	**B06[Cl-Br]**	Presence/absence of Cl - Br at topological distance 6	2D Atom Pairs
3761	**B06[Cl-I]**	Presence/absence of Cl - I at topological distance 6	2D Atom Pairs
3762	**B06[Cl-B]**	Presence/absence of Cl - B at topological distance 6	2D Atom Pairs
3763	**B06[Cl-Si]**	Presence/absence of Cl - Si at topological distance 6	2D Atom Pairs
3764	**B06[Cl-X]**	Presence/absence of Cl - X at topological distance 6	2D Atom Pairs
3765	**B06[Br-Br]**	Presence/absence of Br - Br at topological distance 6	2D Atom Pairs
3766	**B06[Br-I]**	Presence/absence of Br - I at topological distance 6	2D Atom Pairs

No.	Name	Description	Block
3767	**B06[Br-B]**	Presence/absence of Br - B at topological distance 6	2D Atom Pairs
3768	**B06[Br-Si]**	Presence/absence of Br - Si at topological distance 6	2D Atom Pairs
3769	**B06[Br-X]**	Presence/absence of Br - X at topological distance 6	2D Atom Pairs
3770	**B06[I-I]**	Presence/absence of I - I at topological distance 6	2D Atom Pairs
3771	**B06[I-B]**	Presence/absence of I - B at topological distance 6	2D Atom Pairs
3772	**B06[I-Si]**	Presence/absence of I - Si at topological distance 6	2D Atom Pairs
3773	**B06[I-X]**	Presence/absence of I - X at topological distance 6	2D Atom Pairs
3774	**B06[B-B]**	Presence/absence of B - B at topological distance 6	2D Atom Pairs
3775	**B06[B-Si]**	Presence/absence of B - Si at topological distance 6	2D Atom Pairs
3776	**B06[B-X]**	Presence/absence of B - X at topological distance 6	2D Atom Pairs
3777	**B06[Si-Si]**	Presence/absence of Si - Si at topological distance 6	2D Atom Pairs
3778	**B06[Si-X]**	Presence/absence of Si - X at topological distance 6	2D Atom Pairs
3779	**B06[X-X]**	Presence/absence of X - X at topological distance 6	2D Atom Pairs
3780	**B07[C-C]**	Presence/absence of C - C at topological distance 7	2D Atom Pairs
3781	**B07[C-N]**	Presence/absence of C - N at topological distance 7	2D Atom Pairs
3782	**B07[C-O]**	Presence/absence of C - O at topological distance 7	2D Atom Pairs
3783	**B07[C-S]**	Presence/absence of C - S at topological distance 7	2D Atom Pairs
3784	**B07[C-P]**	Presence/absence of C - P at topological distance 7	2D Atom Pairs
3785	**B07[C-F]**	Presence/absence of C - F at topological distance 7	2D Atom Pairs
3786	**B07[C-Cl]**	Presence/absence of C - Cl at topological distance 7	2D Atom Pairs
3787	**B07[C-Br]**	Presence/absence of C - Br at topological distance 7	2D Atom Pairs
3788	**B07[C-I]**	Presence/absence of C - I at topological distance 7	2D Atom Pairs
3789	**B07[C-B]**	Presence/absence of C - B at topological distance 7	2D Atom Pairs
3790	**B07[C-Si]**	Presence/absence of C - Si at topological distance 7	2D Atom Pairs
3791	**B07[C-X]**	Presence/absence of C - X at topological distance 7	2D Atom Pairs
3792	**B07[N-N]**	Presence/absence of N - N at topological distance 7	2D Atom Pairs
3793	**B07[N-O]**	Presence/absence of N - O at topological distance 7	2D Atom Pairs
3794	**B07[N-S]**	Presence/absence of N - S at topological distance 7	2D Atom Pairs
3795	**B07[N-P]**	Presence/absence of N - P at topological distance 7	2D Atom Pairs
3796	**B07[N-F]**	Presence/absence of N - F at topological distance 7	2D Atom Pairs
3797	**B07[N-Cl]**	Presence/absence of N - Cl at topological distance 7	2D Atom Pairs
3798	**B07[N-Br]**	Presence/absence of N - Br at topological distance 7	2D Atom Pairs

No.	Name	Description	Block
3799	**B07[N-I]**	Presence/absence of N - I at topological distance 7	2D Atom Pairs
3800	**B07[N-B]**	Presence/absence of N - B at topological distance 7	2D Atom Pairs
3801	**B07[N-Si]**	Presence/absence of N - Si at topological distance 7	2D Atom Pairs
3802	**B07[N-X]**	Presence/absence of N - X at topological distance 7	2D Atom Pairs
3803	**B07[O-O]**	Presence/absence of O - O at topological distance 7	2D Atom Pairs
3804	**B07[O-S]**	Presence/absence of O - S at topological distance 7	2D Atom Pairs
3805	**B07[O-P]**	Presence/absence of O - P at topological distance 7	2D Atom Pairs
3806	**B07[O-F]**	Presence/absence of O - F at topological distance 7	2D Atom Pairs
3807	**B07[O-Cl]**	Presence/absence of O - Cl at topological distance 7	2D Atom Pairs
3808	**B07[O-Br]**	Presence/absence of O - Br at topological distance 7	2D Atom Pairs
3809	**B07[O-I]**	Presence/absence of O - I at topological distance 7	2D Atom Pairs
3810	**B07[O-B]**	Presence/absence of O - B at topological distance 7	2D Atom Pairs
3811	**B07[O-Si]**	Presence/absence of O - Si at topological distance 7	2D Atom Pairs
3812	**B07[O-X]**	Presence/absence of O - X at topological distance 7	2D Atom Pairs
3813	**B07[S-S]**	Presence/absence of S - S at topological distance 7	2D Atom Pairs
3814	**B07[S-P]**	Presence/absence of S - P at topological distance 7	2D Atom Pairs
3815	**B07[S-F]**	Presence/absence of S - F at topological distance 7	2D Atom Pairs
3816	**B07[S-Cl]**	Presence/absence of S - Cl at topological distance 7	2D Atom Pairs
3817	**B07[S-Br]**	Presence/absence of S - Br at topological distance 7	2D Atom Pairs
3818	**B07[S-I]**	Presence/absence of S - I at topological distance 7	2D Atom Pairs
3819	**B07[S-B]**	Presence/absence of S - B at topological distance 7	2D Atom Pairs
3820	**B07[S-Si]**	Presence/absence of S - Si at topological distance 7	2D Atom Pairs
3821	**B07[S-X]**	Presence/absence of S - X at topological distance 7	2D Atom Pairs
3822	**B07[P-P]**	Presence/absence of P - P at topological distance 7	2D Atom Pairs
3823	**B07[P-F]**	Presence/absence of P - F at topological distance 7	2D Atom Pairs
3824	**B07[P-Cl]**	Presence/absence of P - Cl at topological distance 7	2D Atom Pairs
3825	**B07[P-Br]**	Presence/absence of P - Br at topological distance 7	2D Atom Pairs
3826	**B07[P-I]**	Presence/absence of P - I at topological distance 7	2D Atom Pairs
3827	**B07[P-B]**	Presence/absence of P - B at topological distance 7	2D Atom Pairs
3828	**B07[P-Si]**	Presence/absence of P - Si at topological distance 7	2D Atom Pairs
3829	**B07[P-X]**	Presence/absence of P - X at topological distance 7	2D Atom Pairs
3830	**B07[F-F]**	Presence/absence of F - F at topological distance 7	2D Atom Pairs

No.	Name	Description	Block
3831	**B07[F-Cl]**	Presence/absence of F - Cl at topological distance 7	2D Atom Pairs
3832	**B07[F-Br]**	Presence/absence of F - Br at topological distance 7	2D Atom Pairs
3833	**B07[F-I]**	Presence/absence of F - I at topological distance 7	2D Atom Pairs
3834	**B07[F-B]**	Presence/absence of F - B at topological distance 7	2D Atom Pairs
3835	**B07[F-Si]**	Presence/absence of F - Si at topological distance 7	2D Atom Pairs
3836	**B07[F-X]**	Presence/absence of F - X at topological distance 7	2D Atom Pairs
3837	**B07[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 7	2D Atom Pairs
3838	**B07[Cl-Br]**	Presence/absence of Cl - Br at topological distance 7	2D Atom Pairs
3839	**B07[Cl-I]**	Presence/absence of Cl - I at topological distance 7	2D Atom Pairs
3840	**B07[Cl-B]**	Presence/absence of Cl - B at topological distance 7	2D Atom Pairs
3841	**B07[Cl-Si]**	Presence/absence of Cl - Si at topological distance 7	2D Atom Pairs
3842	**B07[Cl-X]**	Presence/absence of Cl - X at topological distance 7	2D Atom Pairs
3843	**B07[Br-Br]**	Presence/absence of Br - Br at topological distance 7	2D Atom Pairs
3844	**B07[Br-I]**	Presence/absence of Br - I at topological distance 7	2D Atom Pairs
3845	**B07[Br-B]**	Presence/absence of Br - B at topological distance 7	2D Atom Pairs
3846	**B07[Br-Si]**	Presence/absence of Br - Si at topological distance 7	2D Atom Pairs
3847	**B07[Br-X]**	Presence/absence of Br - X at topological distance 7	2D Atom Pairs
3848	**B07[I-I]**	Presence/absence of I - I at topological distance 7	2D Atom Pairs
3849	**B07[I-B]**	Presence/absence of I - B at topological distance 7	2D Atom Pairs
3850	**B07[I-Si]**	Presence/absence of I - Si at topological distance 7	2D Atom Pairs
3851	**B07[I-X]**	Presence/absence of I - X at topological distance 7	2D Atom Pairs
3852	**B07[B-B]**	Presence/absence of B - B at topological distance 7	2D Atom Pairs
3853	**B07[B-Si]**	Presence/absence of B - Si at topological distance 7	2D Atom Pairs
3854	**B07[B-X]**	Presence/absence of B - X at topological distance 7	2D Atom Pairs
3855	**B07[Si-Si]**	Presence/absence of Si - Si at topological distance 7	2D Atom Pairs
3856	**B07[Si-X]**	Presence/absence of Si - X at topological distance 7	2D Atom Pairs
3857	**B07[X-X]**	Presence/absence of X - X at topological distance 7	2D Atom Pairs
3858	**B08[C-C]**	Presence/absence of C - C at topological distance 8	2D Atom Pairs
3859	**B08[C-N]**	Presence/absence of C - N at topological distance 8	2D Atom Pairs
3860	**B08[C-O]**	Presence/absence of C - O at topological distance 8	2D Atom Pairs
3861	**B08[C-S]**	Presence/absence of C - S at topological distance 8	2D Atom Pairs
3862	**B08[C-P]**	Presence/absence of C - P at topological distance 8	2D Atom Pairs

No.	Name	Description	Block
3863	**B08[C-F]**	Presence/absence of C - F at topological distance 8	2D Atom Pairs
3864	**B08[C-Cl]**	Presence/absence of C - Cl at topological distance 8	2D Atom Pairs
3865	**B08[C-Br]**	Presence/absence of C - Br at topological distance 8	2D Atom Pairs
3866	**B08[C-I]**	Presence/absence of C - I at topological distance 8	2D Atom Pairs
3867	**B08[C-B]**	Presence/absence of C - B at topological distance 8	2D Atom Pairs
3868	**B08[C-Si]**	Presence/absence of C - Si at topological distance 8	2D Atom Pairs
3869	**B08[C-X]**	Presence/absence of C - X at topological distance 8	2D Atom Pairs
3870	**B08[N-N]**	Presence/absence of N - N at topological distance 8	2D Atom Pairs
3871	**B08[N-O]**	Presence/absence of N - O at topological distance 8	2D Atom Pairs
3872	**B08[N-S]**	Presence/absence of N - S at topological distance 8	2D Atom Pairs
3873	**B08[N-P]**	Presence/absence of N - P at topological distance 8	2D Atom Pairs
3874	**B08[N-F]**	Presence/absence of N - F at topological distance 8	2D Atom Pairs
3875	**B08[N-Cl]**	Presence/absence of N - Cl at topological distance 8	2D Atom Pairs
3876	**B08[N-Br]**	Presence/absence of N - Br at topological distance 8	2D Atom Pairs
3877	**B08[N-I]**	Presence/absence of N - I at topological distance 8	2D Atom Pairs
3878	**B08[N-B]**	Presence/absence of N - B at topological distance 8	2D Atom Pairs
3879	**B08[N-Si]**	Presence/absence of N - Si at topological distance 8	2D Atom Pairs
3880	**B08[N-X]**	Presence/absence of N - X at topological distance 8	2D Atom Pairs
3881	**B08[O-O]**	Presence/absence of O - O at topological distance 8	2D Atom Pairs
3882	**B08[O-S]**	Presence/absence of O - S at topological distance 8	2D Atom Pairs
3883	**B08[O-P]**	Presence/absence of O - P at topological distance 8	2D Atom Pairs
3884	**B08[O-F]**	Presence/absence of O - F at topological distance 8	2D Atom Pairs
3885	**B08[O-Cl]**	Presence/absence of O - Cl at topological distance 8	2D Atom Pairs
3886	**B08[O-Br]**	Presence/absence of O - Br at topological distance 8	2D Atom Pairs
3887	**B08[O-I]**	Presence/absence of O - I at topological distance 8	2D Atom Pairs
3888	**B08[O-B]**	Presence/absence of O - B at topological distance 8	2D Atom Pairs
3889	**B08[O-Si]**	Presence/absence of O - Si at topological distance 8	2D Atom Pairs
3890	**B08[O-X]**	Presence/absence of O - X at topological distance 8	2D Atom Pairs
3891	**B08[S-S]**	Presence/absence of S - S at topological distance 8	2D Atom Pairs
3892	**B08[S-P]**	Presence/absence of S - P at topological distance 8	2D Atom Pairs
3893	**B08[S-F]**	Presence/absence of S - F at topological distance 8	2D Atom Pairs
3894	**B08[S-Cl]**	Presence/absence of S - Cl at topological distance 8	2D Atom Pairs

No.	Name	Description	Block
3895	**B08[S-Br]**	Presence/absence of S - Br at topological distance 8	2D Atom Pairs
3896	**B08[S-I]**	Presence/absence of S - I at topological distance 8	2D Atom Pairs
3897	**B08[S-B]**	Presence/absence of S - B at topological distance 8	2D Atom Pairs
3898	**B08[S-Si]**	Presence/absence of S - Si at topological distance 8	2D Atom Pairs
3899	**B08[S-X]**	Presence/absence of S - X at topological distance 8	2D Atom Pairs
3900	**B08[P-P]**	Presence/absence of P - P at topological distance 8	2D Atom Pairs
3901	**B08[P-F]**	Presence/absence of P - F at topological distance 8	2D Atom Pairs
3902	**B08[P-Cl]**	Presence/absence of P - Cl at topological distance 8	2D Atom Pairs
3903	**B08[P-Br]**	Presence/absence of P - Br at topological distance 8	2D Atom Pairs
3904	**B08[P-I]**	Presence/absence of P - I at topological distance 8	2D Atom Pairs
3905	**B08[P-B]**	Presence/absence of P - B at topological distance 8	2D Atom Pairs
3906	**B08[P-Si]**	Presence/absence of P - Si at topological distance 8	2D Atom Pairs
3907	**B08[P-X]**	Presence/absence of P - X at topological distance 8	2D Atom Pairs
3908	**B08[F-F]**	Presence/absence of F - F at topological distance 8	2D Atom Pairs
3909	**B08[F-Cl]**	Presence/absence of F - Cl at topological distance 8	2D Atom Pairs
3910	**B08[F-Br]**	Presence/absence of F - Br at topological distance 8	2D Atom Pairs
3911	**B08[F-I]**	Presence/absence of F - I at topological distance 8	2D Atom Pairs
3912	**B08[F-B]**	Presence/absence of F - B at topological distance 8	2D Atom Pairs
3913	**B08[F-Si]**	Presence/absence of F - Si at topological distance 8	2D Atom Pairs
3914	**B08[F-X]**	Presence/absence of F - X at topological distance 8	2D Atom Pairs
3915	**B08[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 8	2D Atom Pairs
3916	**B08[Cl-Br]**	Presence/absence of Cl - Br at topological distance 8	2D Atom Pairs
3917	**B08[Cl-I]**	Presence/absence of Cl - I at topological distance 8	2D Atom Pairs
3918	**B08[Cl-B]**	Presence/absence of Cl - B at topological distance 8	2D Atom Pairs
3919	**B08[Cl-Si]**	Presence/absence of Cl - Si at topological distance 8	2D Atom Pairs
3920	**B08[Cl-X]**	Presence/absence of Cl - X at topological distance 8	2D Atom Pairs
3921	**B08[Br-Br]**	Presence/absence of Br - Br at topological distance 8	2D Atom Pairs
3922	**B08[Br-I]**	Presence/absence of Br - I at topological distance 8	2D Atom Pairs
3923	**B08[Br-B]**	Presence/absence of Br - B at topological distance 8	2D Atom Pairs
3924	**B08[Br-Si]**	Presence/absence of Br - Si at topological distance 8	2D Atom Pairs
3925	**B08[Br-X]**	Presence/absence of Br - X at topological distance 8	2D Atom Pairs
3926	**B08[I-I]**	Presence/absence of I - I at topological distance 8	2D Atom Pairs

No.	Name	Description	Block
3927	**B08[I-B]**	Presence/absence of I - B at topological distance 8	2D Atom Pairs
3928	**B08[I-Si]**	Presence/absence of I - Si at topological distance 8	2D Atom Pairs
3929	**B08[I-X]**	Presence/absence of I - X at topological distance 8	2D Atom Pairs
3930	**B08[B-B]**	Presence/absence of B - B at topological distance 8	2D Atom Pairs
3931	**B08[B-Si]**	Presence/absence of B - Si at topological distance 8	2D Atom Pairs
3932	**B08[B-X]**	Presence/absence of B - X at topological distance 8	2D Atom Pairs
3933	**B08[Si-Si]**	Presence/absence of Si - Si at topological distance 8	2D Atom Pairs
3934	**B08[Si-X]**	Presence/absence of Si - X at topological distance 8	2D Atom Pairs
3935	**B08[X-X]**	Presence/absence of X - X at topological distance 8	2D Atom Pairs
3936	**B09[C-C]**	Presence/absence of C - C at topological distance 9	2D Atom Pairs
3937	**B09[C-N]**	Presence/absence of C - N at topological distance 9	2D Atom Pairs
3938	**B09[C-O]**	Presence/absence of C - O at topological distance 9	2D Atom Pairs
3939	**B09[C-S]**	Presence/absence of C - S at topological distance 9	2D Atom Pairs
3940	**B09[C-P]**	Presence/absence of C - P at topological distance 9	2D Atom Pairs
3941	**B09[C-F]**	Presence/absence of C - F at topological distance 9	2D Atom Pairs
3942	**B09[C-Cl]**	Presence/absence of C - Cl at topological distance 9	2D Atom Pairs
3943	**B09[C-Br]**	Presence/absence of C - Br at topological distance 9	2D Atom Pairs
3944	**B09[C-I]**	Presence/absence of C - I at topological distance 9	2D Atom Pairs
3945	**B09[C-B]**	Presence/absence of C - B at topological distance 9	2D Atom Pairs
3946	**B09[C-Si]**	Presence/absence of C - Si at topological distance 9	2D Atom Pairs
3947	**B09[C-X]**	Presence/absence of C - X at topological distance 9	2D Atom Pairs
3948	**B09[N-N]**	Presence/absence of N - N at topological distance 9	2D Atom Pairs
3949	**B09[N-O]**	Presence/absence of N - O at topological distance 9	2D Atom Pairs
3950	**B09[N-S]**	Presence/absence of N - S at topological distance 9	2D Atom Pairs
3951	**B09[N-P]**	Presence/absence of N - P at topological distance 9	2D Atom Pairs
3952	**B09[N-F]**	Presence/absence of N - F at topological distance 9	2D Atom Pairs
3953	**B09[N-Cl]**	Presence/absence of N - Cl at topological distance 9	2D Atom Pairs
3954	**B09[N-Br]**	Presence/absence of N - Br at topological distance 9	2D Atom Pairs
3955	**B09[N-I]**	Presence/absence of N - I at topological distance 9	2D Atom Pairs
3956	**B09[N-B]**	Presence/absence of N - B at topological distance 9	2D Atom Pairs
3957	**B09[N-Si]**	Presence/absence of N - Si at topological distance 9	2D Atom Pairs
3958	**B09[N-X]**	Presence/absence of N - X at topological distance 9	2D Atom Pairs

No.	Name	Description	Block
3959	**B09[O-O]**	Presence/absence of O - O at topological distance 9	2D Atom Pairs
3960	**B09[O-S]**	Presence/absence of O - S at topological distance 9	2D Atom Pairs
3961	**B09[O-P]**	Presence/absence of O - P at topological distance 9	2D Atom Pairs
3962	**B09[O-F]**	Presence/absence of O - F at topological distance 9	2D Atom Pairs
3963	**B09[O-Cl]**	Presence/absence of O - Cl at topological distance 9	2D Atom Pairs
3964	**B09[O-Br]**	Presence/absence of O - Br at topological distance 9	2D Atom Pairs
3965	**B09[O-I]**	Presence/absence of O - I at topological distance 9	2D Atom Pairs
3966	**B09[O-B]**	Presence/absence of O - B at topological distance 9	2D Atom Pairs
3967	**B09[O-Si]**	Presence/absence of O - Si at topological distance 9	2D Atom Pairs
3968	**B09[O-X]**	Presence/absence of O - X at topological distance 9	2D Atom Pairs
3969	**B09[S-S]**	Presence/absence of S - S at topological distance 9	2D Atom Pairs
3970	**B09[S-P]**	Presence/absence of S - P at topological distance 9	2D Atom Pairs
3971	**B09[S-F]**	Presence/absence of S - F at topological distance 9	2D Atom Pairs
3972	**B09[S-Cl]**	Presence/absence of S - Cl at topological distance 9	2D Atom Pairs
3973	**B09[S-Br]**	Presence/absence of S - Br at topological distance 9	2D Atom Pairs
3974	**B09[S-I]**	Presence/absence of S - I at topological distance 9	2D Atom Pairs
3975	**B09[S-B]**	Presence/absence of S - B at topological distance 9	2D Atom Pairs
3976	**B09[S-Si]**	Presence/absence of S - Si at topological distance 9	2D Atom Pairs
3977	**B09[S-X]**	Presence/absence of S - X at topological distance 9	2D Atom Pairs
3978	**B09[P-P]**	Presence/absence of P - P at topological distance 9	2D Atom Pairs
3979	**B09[P-F]**	Presence/absence of P - F at topological distance 9	2D Atom Pairs
3980	**B09[P-Cl]**	Presence/absence of P - Cl at topological distance 9	2D Atom Pairs
3981	**B09[P-Br]**	Presence/absence of P - Br at topological distance 9	2D Atom Pairs
3982	**B09[P-I]**	Presence/absence of P - I at topological distance 9	2D Atom Pairs
3983	**B09[P-B]**	Presence/absence of P - B at topological distance 9	2D Atom Pairs
3984	**B09[P-Si]**	Presence/absence of P - Si at topological distance 9	2D Atom Pairs
3985	**B09[P-X]**	Presence/absence of P - X at topological distance 9	2D Atom Pairs
3986	**B09[F-F]**	Presence/absence of F - F at topological distance 9	2D Atom Pairs
3987	**B09[F-Cl]**	Presence/absence of F - Cl at topological distance 9	2D Atom Pairs
3988	**B09[F-Br]**	Presence/absence of F - Br at topological distance 9	2D Atom Pairs
3989	**B09[F-I]**	Presence/absence of F - I at topological distance 9	2D Atom Pairs
3990	**B09[F-B]**	Presence/absence of F - B at topological distance 9	2D Atom Pairs

No.	Name	Description	Block
3991	**B09[F-Si]**	Presence/absence of F - Si at topological distance 9	2D Atom Pairs
3992	**B09[F-X]**	Presence/absence of F - X at topological distance 9	2D Atom Pairs
3993	**B09[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 9	2D Atom Pairs
3994	**B09[Cl-Br]**	Presence/absence of Cl - Br at topological distance 9	2D Atom Pairs
3995	**B09[Cl-I]**	Presence/absence of Cl - I at topological distance 9	2D Atom Pairs
3996	**B09[Cl-B]**	Presence/absence of Cl - B at topological distance 9	2D Atom Pairs
3997	**B09[Cl-Si]**	Presence/absence of Cl - Si at topological distance 9	2D Atom Pairs
3998	**B09[Cl-X]**	Presence/absence of Cl - X at topological distance 9	2D Atom Pairs
3999	**B09[Br-Br]**	Presence/absence of Br - Br at topological distance 9	2D Atom Pairs
4000	**B09[Br-I]**	Presence/absence of Br - I at topological distance 9	2D Atom Pairs
4001	**B09[Br-B]**	Presence/absence of Br - B at topological distance 9	2D Atom Pairs
4002	**B09[Br-Si]**	Presence/absence of Br - Si at topological distance 9	2D Atom Pairs
4003	**B09[Br-X]**	Presence/absence of Br - X at topological distance 9	2D Atom Pairs
4004	**B09[I-I]**	Presence/absence of I - I at topological distance 9	2D Atom Pairs
4005	**B09[I-B]**	Presence/absence of I - B at topological distance 9	2D Atom Pairs
4006	**B09[I-Si]**	Presence/absence of I - Si at topological distance 9	2D Atom Pairs
4007	**B09[I-X]**	Presence/absence of I - X at topological distance 9	2D Atom Pairs
4008	**B09[B-B]**	Presence/absence of B - B at topological distance 9	2D Atom Pairs
4009	**B09[B-Si]**	Presence/absence of B - Si at topological distance 9	2D Atom Pairs
4010	**B09[B-X]**	Presence/absence of B - X at topological distance 9	2D Atom Pairs
4011	**B09[Si-Si]**	Presence/absence of Si - Si at topological distance 9	2D Atom Pairs
4012	**B09[Si-X]**	Presence/absence of Si - X at topological distance 9	2D Atom Pairs
4013	**B09[X-X]**	Presence/absence of X - X at topological distance 9	2D Atom Pairs
4014	**B10[C-C]**	Presence/absence of C - C at topological distance 10	2D Atom Pairs
4015	**B10[C-N]**	Presence/absence of C - N at topological distance 10	2D Atom Pairs
4016	**B10[C-O]**	Presence/absence of C - O at topological distance 10	2D Atom Pairs
4017	**B10[C-S]**	Presence/absence of C - S at topological distance 10	2D Atom Pairs
4018	**B10[C-P]**	Presence/absence of C - P at topological distance 10	2D Atom Pairs
4019	**B10[C-F]**	Presence/absence of C - F at topological distance 10	2D Atom Pairs
4020	**B10[C-Cl]**	Presence/absence of C - Cl at topological distance 10	2D Atom Pairs
4021	**B10[C-Br]**	Presence/absence of C - Br at topological distance 10	2D Atom Pairs
4022	**B10[C-I]**	Presence/absence of C - I at topological distance 10	2D Atom Pairs

No.	Name	Description	Block
4023	**B10[C-B]**	Presence/absence of C - B at topological distance 10	2D Atom Pairs
4024	**B10[C-Si]**	Presence/absence of C - Si at topological distance 10	2D Atom Pairs
4025	**B10[C-X]**	Presence/absence of C - X at topological distance 10	2D Atom Pairs
4026	**B10[N-N]**	Presence/absence of N - N at topological distance 10	2D Atom Pairs
4027	**B10[N-O]**	Presence/absence of N - O at topological distance 10	2D Atom Pairs
4028	**B10[N-S]**	Presence/absence of N - S at topological distance 10	2D Atom Pairs
4029	**B10[N-P]**	Presence/absence of N - P at topological distance 10	2D Atom Pairs
4030	**B10[N-F]**	Presence/absence of N - F at topological distance 10	2D Atom Pairs
4031	**B10[N-Cl]**	Presence/absence of N - Cl at topological distance 10	2D Atom Pairs
4032	**B10[N-Br]**	Presence/absence of N - Br at topological distance 10	2D Atom Pairs
4033	**B10[N-I]**	Presence/absence of N - I at topological distance 10	2D Atom Pairs
4034	**B10[N-B]**	Presence/absence of N - B at topological distance 10	2D Atom Pairs
4035	**B10[N-Si]**	Presence/absence of N - Si at topological distance 10	2D Atom Pairs
4036	**B10[N-X]**	Presence/absence of N - X at topological distance 10	2D Atom Pairs
4037	**B10[O-O]**	Presence/absence of O - O at topological distance 10	2D Atom Pairs
4038	**B10[O-S]**	Presence/absence of O - S at topological distance 10	2D Atom Pairs
4039	**B10[O-P]**	Presence/absence of O - P at topological distance 10	2D Atom Pairs
4040	**B10[O-F]**	Presence/absence of O - F at topological distance 10	2D Atom Pairs
4041	**B10[O-Cl]**	Presence/absence of O - Cl at topological distance 10	2D Atom Pairs
4042	**B10[O-Br]**	Presence/absence of O - Br at topological distance 10	2D Atom Pairs
4043	**B10[O-I]**	Presence/absence of O - I at topological distance 10	2D Atom Pairs
4044	**B10[O-B]**	Presence/absence of O - B at topological distance 10	2D Atom Pairs
4045	**B10[O-Si]**	Presence/absence of O - Si at topological distance 10	2D Atom Pairs
4046	**B10[O-X]**	Presence/absence of O - X at topological distance 10	2D Atom Pairs
4047	**B10[S-S]**	Presence/absence of S - S at topological distance 10	2D Atom Pairs
4048	**B10[S-P]**	Presence/absence of S - P at topological distance 10	2D Atom Pairs
4049	**B10[S-F]**	Presence/absence of S - F at topological distance 10	2D Atom Pairs
4050	**B10[S-Cl]**	Presence/absence of S - Cl at topological distance 10	2D Atom Pairs
4051	**B10[S-Br]**	Presence/absence of S - Br at topological distance 10	2D Atom Pairs
4052	**B10[S-I]**	Presence/absence of S - I at topological distance 10	2D Atom Pairs
4053	**B10[S-B]**	Presence/absence of S - B at topological distance 10	2D Atom Pairs
4054	**B10[S-Si]**	Presence/absence of S - Si at topological distance 10	2D Atom Pairs

No.	Name	Description	Block
4055	**B10[S-X]**	Presence/absence of S - X at topological distance 10	2D Atom Pairs
4056	**B10[P-P]**	Presence/absence of P - P at topological distance 10	2D Atom Pairs
4057	**B10[P-F]**	Presence/absence of P - F at topological distance 10	2D Atom Pairs
4058	**B10[P-Cl]**	Presence/absence of P - Cl at topological distance 10	2D Atom Pairs
4059	**B10[P-Br]**	Presence/absence of P - Br at topological distance 10	2D Atom Pairs
4060	**B10[P-I]**	Presence/absence of P - I at topological distance 10	2D Atom Pairs
4061	**B10[P-B]**	Presence/absence of P - B at topological distance 10	2D Atom Pairs
4062	**B10[P-Si]**	Presence/absence of P - Si at topological distance 10	2D Atom Pairs
4063	**B10[P-X]**	Presence/absence of P - X at topological distance 10	2D Atom Pairs
4064	**B10[F-F]**	Presence/absence of F - F at topological distance 10	2D Atom Pairs
4065	**B10[F-Cl]**	Presence/absence of F - Cl at topological distance 10	2D Atom Pairs
4066	**B10[F-Br]**	Presence/absence of F - Br at topological distance 10	2D Atom Pairs
4067	**B10[F-I]**	Presence/absence of F - I at topological distance 10	2D Atom Pairs
4068	**B10[F-B]**	Presence/absence of F - B at topological distance 10	2D Atom Pairs
4069	**B10[F-Si]**	Presence/absence of F - Si at topological distance 10	2D Atom Pairs
4070	**B10[F-X]**	Presence/absence of F - X at topological distance 10	2D Atom Pairs
4071	**B10[Cl-Cl]**	Presence/absence of Cl - Cl at topological distance 10	2D Atom Pairs
4072	**B10[Cl-Br]**	Presence/absence of Cl - Br at topological distance 10	2D Atom Pairs
4073	**B10[Cl-I]**	Presence/absence of Cl - I at topological distance 10	2D Atom Pairs
4074	**B10[Cl-B]**	Presence/absence of Cl - B at topological distance 10	2D Atom Pairs
4075	**B10[Cl-Si]**	Presence/absence of Cl - Si at topological distance 10	2D Atom Pairs
4076	**B10[Cl-X]**	Presence/absence of Cl - X at topological distance 10	2D Atom Pairs
4077	**B10[Br-Br]**	Presence/absence of Br - Br at topological distance 10	2D Atom Pairs
4078	**B10[Br-I]**	Presence/absence of Br - I at topological distance 10	2D Atom Pairs
4079	**B10[Br-B]**	Presence/absence of Br - B at topological distance 10	2D Atom Pairs
4080	**B10[Br-Si]**	Presence/absence of Br - Si at topological distance 10	2D Atom Pairs
4081	**B10[Br-X]**	Presence/absence of Br - X at topological distance 10	2D Atom Pairs
4082	**B10[I-I]**	Presence/absence of I - I at topological distance 10	2D Atom Pairs
4083	**B10[I-B]**	Presence/absence of I - B at topological distance 10	2D Atom Pairs
4084	**B10[I-Si]**	Presence/absence of I - Si at topological distance 10	2D Atom Pairs
4085	**B10[I-X]**	Presence/absence of I - X at topological distance 10	2D Atom Pairs
4086	**B10[B-B]**	Presence/absence of B - B at topological distance 10	2D Atom Pairs

No.	Name	Description	Block
4087	**B10[B-Si]**	Presence/absence of B - Si at topological distance 10	2D Atom Pairs
4088	**B10[B-X]**	Presence/absence of B - X at topological distance 10	2D Atom Pairs
4089	**B10[Si-Si]**	Presence/absence of Si - Si at topological distance 10	2D Atom Pairs
4090	**B10[Si-X]**	Presence/absence of Si - X at topological distance 10	2D Atom Pairs
4091	**B10[X-X]**	Presence/absence of X - X at topological distance 10	2D Atom Pairs
4092	**F01[C-C]**	Frequency of C - C at topological distance 1	2D Atom Pairs
4093	**F01[C-N]**	Frequency of C - N at topological distance 1	2D Atom Pairs
4094	**F01[C-O]**	Frequency of C - O at topological distance 1	2D Atom Pairs
4095	**F01[C-S]**	Frequency of C - S at topological distance 1	2D Atom Pairs
4096	**F01[C-P]**	Frequency of C - P at topological distance 1	2D Atom Pairs
4097	**F01[C-F]**	Frequency of C - F at topological distance 1	2D Atom Pairs
4098	**F01[C-Cl]**	Frequency of C - Cl at topological distance 1	2D Atom Pairs
4099	**F01[C-Br]**	Frequency of C - Br at topological distance 1	2D Atom Pairs
4100	**F01[C-I]**	Frequency of C - I at topological distance 1	2D Atom Pairs
4101	**F01[C-B]**	Frequency of C - B at topological distance 1	2D Atom Pairs
4102	**F01[C-Si]**	Frequency of C - Si at topological distance 1	2D Atom Pairs
4103	**F01[C-X]**	Frequency of C - X at topological distance 1	2D Atom Pairs
4104	**F01[N-N]**	Frequency of N - N at topological distance 1	2D Atom Pairs
4105	**F01[N-O]**	Frequency of N - O at topological distance 1	2D Atom Pairs
4106	**F01[N-S]**	Frequency of N - S at topological distance 1	2D Atom Pairs
4107	**F01[N-P]**	Frequency of N - P at topological distance 1	2D Atom Pairs
4108	**F01[N-F]**	Frequency of N - F at topological distance 1	2D Atom Pairs
4109	**F01[N-Cl]**	Frequency of N - Cl at topological distance 1	2D Atom Pairs
4110	**F01[N-Br]**	Frequency of N - Br at topological distance 1	2D Atom Pairs
4111	**F01[N-I]**	Frequency of N - I at topological distance 1	2D Atom Pairs
4112	**F01[N-B]**	Frequency of N - B at topological distance 1	2D Atom Pairs
4113	**F01[N-Si]**	Frequency of N - Si at topological distance 1	2D Atom Pairs
4114	**F01[N-X]**	Frequency of N - X at topological distance 1	2D Atom Pairs
4115	**F01[O-O]**	Frequency of O - O at topological distance 1	2D Atom Pairs
4116	**F01[O-S]**	Frequency of O - S at topological distance 1	2D Atom Pairs
4117	**F01[O-P]**	Frequency of O - P at topological distance 1	2D Atom Pairs
4118	**F01[O-F]**	Frequency of O - F at topological distance 1	2D Atom Pairs

No.	Name	Description	Block
4119	**F01[O-Cl]**	Frequency of O - Cl at topological distance 1	2D Atom Pairs
4120	**F01[O-Br]**	Frequency of O - Br at topological distance 1	2D Atom Pairs
4121	**F01[O-I]**	Frequency of O - I at topological distance 1	2D Atom Pairs
4122	**F01[O-B]**	Frequency of O - B at topological distance 1	2D Atom Pairs
4123	**F01[O-Si]**	Frequency of O - Si at topological distance 1	2D Atom Pairs
4124	**F01[O-X]**	Frequency of O - X at topological distance 1	2D Atom Pairs
4125	**F01[S-S]**	Frequency of S - S at topological distance 1	2D Atom Pairs
4126	**F01[S-P]**	Frequency of S - P at topological distance 1	2D Atom Pairs
4127	**F01[S-F]**	Frequency of S - F at topological distance 1	2D Atom Pairs
4128	**F01[S-Cl]**	Frequency of S - Cl at topological distance 1	2D Atom Pairs
4129	**F01[S-Br]**	Frequency of S - Br at topological distance 1	2D Atom Pairs
4130	**F01[S-I]**	Frequency of S - I at topological distance 1	2D Atom Pairs
4131	**F01[S-B]**	Frequency of S - B at topological distance 1	2D Atom Pairs
4132	**F01[S-Si]**	Frequency of S - Si at topological distance 1	2D Atom Pairs
4133	**F01[S-X]**	Frequency of S - X at topological distance 1	2D Atom Pairs
4134	**F01[P-P]**	Frequency of P - P at topological distance 1	2D Atom Pairs
4135	**F01[P-F]**	Frequency of P - F at topological distance 1	2D Atom Pairs
4136	**F01[P-Cl]**	Frequency of P - Cl at topological distance 1	2D Atom Pairs
4137	**F01[P-Br]**	Frequency of P - Br at topological distance 1	2D Atom Pairs
4138	**F01[P-I]**	Frequency of P - I at topological distance 1	2D Atom Pairs
4139	**F01[P-B]**	Frequency of P - B at topological distance 1	2D Atom Pairs
4140	**F01[P-Si]**	Frequency of P - Si at topological distance 1	2D Atom Pairs
4141	**F01[P-X]**	Frequency of P - X at topological distance 1	2D Atom Pairs
4142	**F01[F-F]**	Frequency of F - F at topological distance 1	2D Atom Pairs
4143	**F01[F-Cl]**	Frequency of F - Cl at topological distance 1	2D Atom Pairs
4144	**F01[F-Br]**	Frequency of F - Br at topological distance 1	2D Atom Pairs
4145	**F01[F-I]**	Frequency of F - I at topological distance 1	2D Atom Pairs
4146	**F01[F-B]**	Frequency of F - B at topological distance 1	2D Atom Pairs
4147	**F01[F-Si]**	Frequency of F - Si at topological distance 1	2D Atom Pairs
4148	**F01[F-X]**	Frequency of F - X at topological distance 1	2D Atom Pairs
4149	**F01[Cl-Cl]**	Frequency of Cl - Cl at topological distance 1	2D Atom Pairs
4150	**F01[Cl-Br]**	Frequency of Cl - Br at topological distance 1	2D Atom Pairs

No.	Name	Description	Block
4151	**F01[Cl-I]**	Frequency of Cl - I at topological distance 1	2D Atom Pairs
4152	**F01[Cl-B]**	Frequency of Cl - B at topological distance 1	2D Atom Pairs
4153	**F01[Cl-Si]**	Frequency of Cl - Si at topological distance 1	2D Atom Pairs
4154	**F01[Cl-X]**	Frequency of Cl - X at topological distance 1	2D Atom Pairs
4155	**F01[Br-Br]**	Frequency of Br - Br at topological distance 1	2D Atom Pairs
4156	**F01[Br-I]**	Frequency of Br - I at topological distance 1	2D Atom Pairs
4157	**F01[Br-B]**	Frequency of Br - B at topological distance 1	2D Atom Pairs
4158	**F01[Br-Si]**	Frequency of Br - Si at topological distance 1	2D Atom Pairs
4159	**F01[Br-X]**	Frequency of Br - X at topological distance 1	2D Atom Pairs
4160	**F01[I-I]**	Frequency of I - I at topological distance 1	2D Atom Pairs
4161	**F01[I-B]**	Frequency of I - B at topological distance 1	2D Atom Pairs
4162	**F01[I-Si]**	Frequency of I - Si at topological distance 1	2D Atom Pairs
4163	**F01[I-X]**	Frequency of I - X at topological distance 1	2D Atom Pairs
4164	**F01[B-B]**	Frequency of B - B at topological distance 1	2D Atom Pairs
4165	**F01[B-Si]**	Frequency of B - Si at topological distance 1	2D Atom Pairs
4166	**F01[B-X]**	Frequency of B - X at topological distance 1	2D Atom Pairs
4167	**F01[Si-Si]**	Frequency of Si - Si at topological distance 1	2D Atom Pairs
4168	**F01[Si-X]**	Frequency of Si - X at topological distance 1	2D Atom Pairs
4169	**F01[X-X]**	Frequency of X - X at topological distance 1	2D Atom Pairs
4170	**F02[C-C]**	Frequency of C - C at topological distance 2	2D Atom Pairs
4171	**F02[C-N]**	Frequency of C - N at topological distance 2	2D Atom Pairs
4172	**F02[C-O]**	Frequency of C - O at topological distance 2	2D Atom Pairs
4173	**F02[C-S]**	Frequency of C - S at topological distance 2	2D Atom Pairs
4174	**F02[C-P]**	Frequency of C - P at topological distance 2	2D Atom Pairs
4175	**F02[C-F]**	Frequency of C - F at topological distance 2	2D Atom Pairs
4176	**F02[C-Cl]**	Frequency of C - Cl at topological distance 2	2D Atom Pairs
4177	**F02[C-Br]**	Frequency of C - Br at topological distance 2	2D Atom Pairs
4178	**F02[C-I]**	Frequency of C - I at topological distance 2	2D Atom Pairs
4179	**F02[C-B]**	Frequency of C - B at topological distance 2	2D Atom Pairs
4180	**F02[C-Si]**	Frequency of C - Si at topological distance 2	2D Atom Pairs
4181	**F02[C-X]**	Frequency of C - X at topological distance 2	2D Atom Pairs
4182	**F02[N-N]**	Frequency of N - N at topological distance 2	2D Atom Pairs

No.	Name	Description	Block
4183	**F02[N-O]**	Frequency of N - O at topological distance 2	2D Atom Pairs
4184	**F02[N-S]**	Frequency of N - S at topological distance 2	2D Atom Pairs
4185	**F02[N-P]**	Frequency of N - P at topological distance 2	2D Atom Pairs
4186	**F02[N-F]**	Frequency of N - F at topological distance 2	2D Atom Pairs
4187	**F02[N-Cl]**	Frequency of N - Cl at topological distance 2	2D Atom Pairs
4188	**F02[N-Br]**	Frequency of N - Br at topological distance 2	2D Atom Pairs
4189	**F02[N-I]**	Frequency of N - I at topological distance 2	2D Atom Pairs
4190	**F02[N-B]**	Frequency of N - B at topological distance 2	2D Atom Pairs
4191	**F02[N-Si]**	Frequency of N - Si at topological distance 2	2D Atom Pairs
4192	**F02[N-X]**	Frequency of N - X at topological distance 2	2D Atom Pairs
4193	**F02[O-O]**	Frequency of O - O at topological distance 2	2D Atom Pairs
4194	**F02[O-S]**	Frequency of O - S at topological distance 2	2D Atom Pairs
4195	**F02[O-P]**	Frequency of O - P at topological distance 2	2D Atom Pairs
4196	**F02[O-F]**	Frequency of O - F at topological distance 2	2D Atom Pairs
4197	**F02[O-Cl]**	Frequency of O - Cl at topological distance 2	2D Atom Pairs
4198	**F02[O-Br]**	Frequency of O - Br at topological distance 2	2D Atom Pairs
4199	**F02[O-I]**	Frequency of O - I at topological distance 2	2D Atom Pairs
4200	**F02[O-B]**	Frequency of O - B at topological distance 2	2D Atom Pairs
4201	**F02[O-Si]**	Frequency of O - Si at topological distance 2	2D Atom Pairs
4202	**F02[O-X]**	Frequency of O - X at topological distance 2	2D Atom Pairs
4203	**F02[S-S]**	Frequency of S - S at topological distance 2	2D Atom Pairs
4204	**F02[S-P]**	Frequency of S - P at topological distance 2	2D Atom Pairs
4205	**F02[S-F]**	Frequency of S - F at topological distance 2	2D Atom Pairs
4206	**F02[S-Cl]**	Frequency of S - Cl at topological distance 2	2D Atom Pairs
4207	**F02[S-Br]**	Frequency of S - Br at topological distance 2	2D Atom Pairs
4208	**F02[S-I]**	Frequency of S - I at topological distance 2	2D Atom Pairs
4209	**F02[S-B]**	Frequency of S - B at topological distance 2	2D Atom Pairs
4210	**F02[S-Si]**	Frequency of S - Si at topological distance 2	2D Atom Pairs
4211	**F02[S-X]**	Frequency of S - X at topological distance 2	2D Atom Pairs
4212	**F02[P-P]**	Frequency of P - P at topological distance 2	2D Atom Pairs
4213	**F02[P-F]**	Frequency of P - F at topological distance 2	2D Atom Pairs
4214	**F02[P-Cl]**	Frequency of P - Cl at topological distance 2	2D Atom Pairs

No.	Name	Description	Block
4215	**F02[P-Br]**	Frequency of P - Br at topological distance 2	2D Atom Pairs
4216	**F02[P-I]**	Frequency of P - I at topological distance 2	2D Atom Pairs
4217	**F02[P-B]**	Frequency of P - B at topological distance 2	2D Atom Pairs
4218	**F02[P-Si]**	Frequency of P - Si at topological distance 2	2D Atom Pairs
4219	**F02[P-X]**	Frequency of P - X at topological distance 2	2D Atom Pairs
4220	**F02[F-F]**	Frequency of F - F at topological distance 2	2D Atom Pairs
4221	**F02[F-Cl]**	Frequency of F - Cl at topological distance 2	2D Atom Pairs
4222	**F02[F-Br]**	Frequency of F - Br at topological distance 2	2D Atom Pairs
4223	**F02[F-I]**	Frequency of F - I at topological distance 2	2D Atom Pairs
4224	**F02[F-B]**	Frequency of F - B at topological distance 2	2D Atom Pairs
4225	**F02[F-Si]**	Frequency of F - Si at topological distance 2	2D Atom Pairs
4226	**F02[F-X]**	Frequency of F - X at topological distance 2	2D Atom Pairs
4227	**F02[Cl-Cl]**	Frequency of Cl - Cl at topological distance 2	2D Atom Pairs
4228	**F02[Cl-Br]**	Frequency of Cl - Br at topological distance 2	2D Atom Pairs
4229	**F02[Cl-I]**	Frequency of Cl - I at topological distance 2	2D Atom Pairs
4230	**F02[Cl-B]**	Frequency of Cl - B at topological distance 2	2D Atom Pairs
4231	**F02[Cl-Si]**	Frequency of Cl - Si at topological distance 2	2D Atom Pairs
4232	**F02[Cl-X]**	Frequency of Cl - X at topological distance 2	2D Atom Pairs
4233	**F02[Br-Br]**	Frequency of Br - Br at topological distance 2	2D Atom Pairs
4234	**F02[Br-I]**	Frequency of Br - I at topological distance 2	2D Atom Pairs
4235	**F02[Br-B]**	Frequency of Br - B at topological distance 2	2D Atom Pairs
4236	**F02[Br-Si]**	Frequency of Br - Si at topological distance 2	2D Atom Pairs
4237	**F02[Br-X]**	Frequency of Br - X at topological distance 2	2D Atom Pairs
4238	**F02[I-I]**	Frequency of I - I at topological distance 2	2D Atom Pairs
4239	**F02[I-B]**	Frequency of I - B at topological distance 2	2D Atom Pairs
4240	**F02[I-Si]**	Frequency of I - Si at topological distance 2	2D Atom Pairs
4241	**F02[I-X]**	Frequency of I - X at topological distance 2	2D Atom Pairs
4242	**F02[B-B]**	Frequency of B - B at topological distance 2	2D Atom Pairs
4243	**F02[B-Si]**	Frequency of B - Si at topological distance 2	2D Atom Pairs
4244	**F02[B-X]**	Frequency of B - X at topological distance 2	2D Atom Pairs
4245	**F02[Si-Si]**	Frequency of Si - Si at topological distance 2	2D Atom Pairs
4246	**F02[Si-X]**	Frequency of Si - X at topological distance 2	2D Atom Pairs

No.	Name	Description	Block
4247	**F02[X-X]**	Frequency of X - X at topological distance 2	2D Atom Pairs
4248	**F03[C-C]**	Frequency of C - C at topological distance 3	2D Atom Pairs
4249	**F03[C-N]**	Frequency of C - N at topological distance 3	2D Atom Pairs
4250	**F03[C-O]**	Frequency of C - O at topological distance 3	2D Atom Pairs
4251	**F03[C-S]**	Frequency of C - S at topological distance 3	2D Atom Pairs
4252	**F03[C-P]**	Frequency of C - P at topological distance 3	2D Atom Pairs
4253	**F03[C-F]**	Frequency of C - F at topological distance 3	2D Atom Pairs
4254	**F03[C-Cl]**	Frequency of C - Cl at topological distance 3	2D Atom Pairs
4255	**F03[C-Br]**	Frequency of C - Br at topological distance 3	2D Atom Pairs
4256	**F03[C-I]**	Frequency of C - I at topological distance 3	2D Atom Pairs
4257	**F03[C-B]**	Frequency of C - B at topological distance 3	2D Atom Pairs
4258	**F03[C-Si]**	Frequency of C - Si at topological distance 3	2D Atom Pairs
4259	**F03[C-X]**	Frequency of C - X at topological distance 3	2D Atom Pairs
4260	**F03[N-N]**	Frequency of N - N at topological distance 3	2D Atom Pairs
4261	**F03[N-O]**	Frequency of N - O at topological distance 3	2D Atom Pairs
4262	**F03[N-S]**	Frequency of N - S at topological distance 3	2D Atom Pairs
4263	**F03[N-P]**	Frequency of N - P at topological distance 3	2D Atom Pairs
4264	**F03[N-F]**	Frequency of N - F at topological distance 3	2D Atom Pairs
4265	**F03[N-Cl]**	Frequency of N - Cl at topological distance 3	2D Atom Pairs
4266	**F03[N-Br]**	Frequency of N - Br at topological distance 3	2D Atom Pairs
4267	**F03[N-I]**	Frequency of N - I at topological distance 3	2D Atom Pairs
4268	**F03[N-B]**	Frequency of N - B at topological distance 3	2D Atom Pairs
4269	**F03[N-Si]**	Frequency of N - Si at topological distance 3	2D Atom Pairs
4270	**F03[N-X]**	Frequency of N - X at topological distance 3	2D Atom Pairs
4271	**F03[O-O]**	Frequency of O - O at topological distance 3	2D Atom Pairs
4272	**F03[O-S]**	Frequency of O - S at topological distance 3	2D Atom Pairs
4273	**F03[O-P]**	Frequency of O - P at topological distance 3	2D Atom Pairs
4274	**F03[O-F]**	Frequency of O - F at topological distance 3	2D Atom Pairs
4275	**F03[O-Cl]**	Frequency of O - Cl at topological distance 3	2D Atom Pairs
4276	**F03[O-Br]**	Frequency of O - Br at topological distance 3	2D Atom Pairs
4277	**F03[O-I]**	Frequency of O - I at topological distance 3	2D Atom Pairs
4278	**F03[O-B]**	Frequency of O - B at topological distance 3	2D Atom Pairs

No.	Name	Description	Block
4279	**F03[O-Si]**	Frequency of O - Si at topological distance 3	2D Atom Pairs
4280	**F03[O-X]**	Frequency of O - X at topological distance 3	2D Atom Pairs
4281	**F03[S-S]**	Frequency of S - S at topological distance 3	2D Atom Pairs
4282	**F03[S-P]**	Frequency of S - P at topological distance 3	2D Atom Pairs
4283	**F03[S-F]**	Frequency of S - F at topological distance 3	2D Atom Pairs
4284	**F03[S-Cl]**	Frequency of S - Cl at topological distance 3	2D Atom Pairs
4285	**F03[S-Br]**	Frequency of S - Br at topological distance 3	2D Atom Pairs
4286	**F03[S-I]**	Frequency of S - I at topological distance 3	2D Atom Pairs
4287	**F03[S-B]**	Frequency of S - B at topological distance 3	2D Atom Pairs
4288	**F03[S-Si]**	Frequency of S - Si at topological distance 3	2D Atom Pairs
4289	**F03[S-X]**	Frequency of S - X at topological distance 3	2D Atom Pairs
4290	**F03[P-P]**	Frequency of P - P at topological distance 3	2D Atom Pairs
4291	**F03[P-F]**	Frequency of P - F at topological distance 3	2D Atom Pairs
4292	**F03[P-Cl]**	Frequency of P - Cl at topological distance 3	2D Atom Pairs
4293	**F03[P-Br]**	Frequency of P - Br at topological distance 3	2D Atom Pairs
4294	**F03[P-I]**	Frequency of P - I at topological distance 3	2D Atom Pairs
4295	**F03[P-B]**	Frequency of P - B at topological distance 3	2D Atom Pairs
4296	**F03[P-Si]**	Frequency of P - Si at topological distance 3	2D Atom Pairs
4297	**F03[P-X]**	Frequency of P - X at topological distance 3	2D Atom Pairs
4298	**F03[F-F]**	Frequency of F - F at topological distance 3	2D Atom Pairs
4299	**F03[F-Cl]**	Frequency of F - Cl at topological distance 3	2D Atom Pairs
4300	**F03[F-Br]**	Frequency of F - Br at topological distance 3	2D Atom Pairs
4301	**F03[F-I]**	Frequency of F - I at topological distance 3	2D Atom Pairs
4302	**F03[F-B]**	Frequency of F - B at topological distance 3	2D Atom Pairs
4303	**F03[F-Si]**	Frequency of F - Si at topological distance 3	2D Atom Pairs
4304	**F03[F-X]**	Frequency of F - X at topological distance 3	2D Atom Pairs
4305	**F03[Cl-Cl]**	Frequency of Cl - Cl at topological distance 3	2D Atom Pairs
4306	**F03[Cl-Br]**	Frequency of Cl - Br at topological distance 3	2D Atom Pairs
4307	**F03[Cl-I]**	Frequency of Cl - I at topological distance 3	2D Atom Pairs
4308	**F03[Cl-B]**	Frequency of Cl - B at topological distance 3	2D Atom Pairs
4309	**F03[Cl-Si]**	Frequency of Cl - Si at topological distance 3	2D Atom Pairs
4310	**F03[Cl-X]**	Frequency of Cl - X at topological distance 3	2D Atom Pairs

No.	Name	Description	Block
4311	**F03[Br-Br]**	Frequency of Br - Br at topological distance 3	2D Atom Pairs
4312	**F03[Br-I]**	Frequency of Br - I at topological distance 3	2D Atom Pairs
4313	**F03[Br-B]**	Frequency of Br - B at topological distance 3	2D Atom Pairs
4314	**F03[Br-Si]**	Frequency of Br - Si at topological distance 3	2D Atom Pairs
4315	**F03[Br-X]**	Frequency of Br - X at topological distance 3	2D Atom Pairs
4316	**F03[I-I]**	Frequency of I - I at topological distance 3	2D Atom Pairs
4317	**F03[I-B]**	Frequency of I - B at topological distance 3	2D Atom Pairs
4318	**F03[I-Si]**	Frequency of I - Si at topological distance 3	2D Atom Pairs
4319	**F03[I-X]**	Frequency of I - X at topological distance 3	2D Atom Pairs
4320	**F03[B-B]**	Frequency of B - B at topological distance 3	2D Atom Pairs
4321	**F03[B-Si]**	Frequency of B - Si at topological distance 3	2D Atom Pairs
4322	**F03[B-X]**	Frequency of B - X at topological distance 3	2D Atom Pairs
4323	**F03[Si-Si]**	Frequency of Si - Si at topological distance 3	2D Atom Pairs
4324	**F03[Si-X]**	Frequency of Si - X at topological distance 3	2D Atom Pairs
4325	**F03[X-X]**	Frequency of X - X at topological distance 3	2D Atom Pairs
4326	**F04[C-C]**	Frequency of C - C at topological distance 4	2D Atom Pairs
4327	**F04[C-N]**	Frequency of C - N at topological distance 4	2D Atom Pairs
4328	**F04[C-O]**	Frequency of C - O at topological distance 4	2D Atom Pairs
4329	**F04[C-S]**	Frequency of C - S at topological distance 4	2D Atom Pairs
4330	**F04[C-P]**	Frequency of C - P at topological distance 4	2D Atom Pairs
4331	**F04[C-F]**	Frequency of C - F at topological distance 4	2D Atom Pairs
4332	**F04[C-Cl]**	Frequency of C - Cl at topological distance 4	2D Atom Pairs
4333	**F04[C-Br]**	Frequency of C - Br at topological distance 4	2D Atom Pairs
4334	**F04[C-I]**	Frequency of C - I at topological distance 4	2D Atom Pairs
4335	**F04[C-B]**	Frequency of C - B at topological distance 4	2D Atom Pairs
4336	**F04[C-Si]**	Frequency of C - Si at topological distance 4	2D Atom Pairs
4337	**F04[C-X]**	Frequency of C - X at topological distance 4	2D Atom Pairs
4338	**F04[N-N]**	Frequency of N - N at topological distance 4	2D Atom Pairs
4339	**F04[N-O]**	Frequency of N - O at topological distance 4	2D Atom Pairs
4340	**F04[N-S]**	Frequency of N - S at topological distance 4	2D Atom Pairs
4341	**F04[N-P]**	Frequency of N - P at topological distance 4	2D Atom Pairs
4342	**F04[N-F]**	Frequency of N - F at topological distance 4	2D Atom Pairs

No.	Name	Description	Block
4343	**F04[N-Cl]**	Frequency of N - Cl at topological distance 4	2D Atom Pairs
4344	**F04[N-Br]**	Frequency of N - Br at topological distance 4	2D Atom Pairs
4345	**F04[N-I]**	Frequency of N - I at topological distance 4	2D Atom Pairs
4346	**F04[N-B]**	Frequency of N - B at topological distance 4	2D Atom Pairs
4347	**F04[N-Si]**	Frequency of N - Si at topological distance 4	2D Atom Pairs
4348	**F04[N-X]**	Frequency of N - X at topological distance 4	2D Atom Pairs
4349	**F04[O-O]**	Frequency of O - O at topological distance 4	2D Atom Pairs
4350	**F04[O-S]**	Frequency of O - S at topological distance 4	2D Atom Pairs
4351	**F04[O-P]**	Frequency of O - P at topological distance 4	2D Atom Pairs
4352	**F04[O-F]**	Frequency of O - F at topological distance 4	2D Atom Pairs
4353	**F04[O-Cl]**	Frequency of O - Cl at topological distance 4	2D Atom Pairs
4354	**F04[O-Br]**	Frequency of O - Br at topological distance 4	2D Atom Pairs
4355	**F04[O-I]**	Frequency of O - I at topological distance 4	2D Atom Pairs
4356	**F04[O-B]**	Frequency of O - B at topological distance 4	2D Atom Pairs
4357	**F04[O-Si]**	Frequency of O - Si at topological distance 4	2D Atom Pairs
4358	**F04[O-X]**	Frequency of O - X at topological distance 4	2D Atom Pairs
4359	**F04[S-S]**	Frequency of S - S at topological distance 4	2D Atom Pairs
4360	**F04[S-P]**	Frequency of S - P at topological distance 4	2D Atom Pairs
4361	**F04[S-F]**	Frequency of S - F at topological distance 4	2D Atom Pairs
4362	**F04[S-Cl]**	Frequency of S - Cl at topological distance 4	2D Atom Pairs
4363	**F04[S-Br]**	Frequency of S - Br at topological distance 4	2D Atom Pairs
4364	**F04[S-I]**	Frequency of S - I at topological distance 4	2D Atom Pairs
4365	**F04[S-B]**	Frequency of S - B at topological distance 4	2D Atom Pairs
4366	**F04[S-Si]**	Frequency of S - Si at topological distance 4	2D Atom Pairs
4367	**F04[S-X]**	Frequency of S - X at topological distance 4	2D Atom Pairs
4368	**F04[P-P]**	Frequency of P - P at topological distance 4	2D Atom Pairs
4369	**F04[P-F]**	Frequency of P - F at topological distance 4	2D Atom Pairs
4370	**F04[P-Cl]**	Frequency of P - Cl at topological distance 4	2D Atom Pairs
4371	**F04[P-Br]**	Frequency of P - Br at topological distance 4	2D Atom Pairs
4372	**F04[P-I]**	Frequency of P - I at topological distance 4	2D Atom Pairs
4373	**F04[P-B]**	Frequency of P - B at topological distance 4	2D Atom Pairs
4374	**F04[P-Si]**	Frequency of P - Si at topological distance 4	2D Atom Pairs

No.	Name	Description	Block
4375	**F04[P-X]**	Frequency of P - X at topological distance 4	2D Atom Pairs
4376	**F04[F-F]**	Frequency of F - F at topological distance 4	2D Atom Pairs
4377	**F04[F-Cl]**	Frequency of F - Cl at topological distance 4	2D Atom Pairs
4378	**F04[F-Br]**	Frequency of F - Br at topological distance 4	2D Atom Pairs
4379	**F04[F-I]**	Frequency of F - I at topological distance 4	2D Atom Pairs
4380	**F04[F-B]**	Frequency of F - B at topological distance 4	2D Atom Pairs
4381	**F04[F-Si]**	Frequency of F - Si at topological distance 4	2D Atom Pairs
4382	**F04[F-X]**	Frequency of F - X at topological distance 4	2D Atom Pairs
4383	**F04[Cl-Cl]**	Frequency of Cl - Cl at topological distance 4	2D Atom Pairs
4384	**F04[Cl-Br]**	Frequency of Cl - Br at topological distance 4	2D Atom Pairs
4385	**F04[Cl-I]**	Frequency of Cl - I at topological distance 4	2D Atom Pairs
4386	**F04[Cl-B]**	Frequency of Cl - B at topological distance 4	2D Atom Pairs
4387	**F04[Cl-Si]**	Frequency of Cl - Si at topological distance 4	2D Atom Pairs
4388	**F04[Cl-X]**	Frequency of Cl - X at topological distance 4	2D Atom Pairs
4389	**F04[Br-Br]**	Frequency of Br - Br at topological distance 4	2D Atom Pairs
4390	**F04[Br-I]**	Frequency of Br - I at topological distance 4	2D Atom Pairs
4391	**F04[Br-B]**	Frequency of Br - B at topological distance 4	2D Atom Pairs
4392	**F04[Br-Si]**	Frequency of Br - Si at topological distance 4	2D Atom Pairs
4393	**F04[Br-X]**	Frequency of Br - X at topological distance 4	2D Atom Pairs
4394	**F04[I-I]**	Frequency of I - I at topological distance 4	2D Atom Pairs
4395	**F04[I-B]**	Frequency of I - B at topological distance 4	2D Atom Pairs
4396	**F04[I-Si]**	Frequency of I - Si at topological distance 4	2D Atom Pairs
4397	**F04[I-X]**	Frequency of I - X at topological distance 4	2D Atom Pairs
4398	**F04[B-B]**	Frequency of B - B at topological distance 4	2D Atom Pairs
4399	**F04[B-Si]**	Frequency of B - Si at topological distance 4	2D Atom Pairs
4400	**F04[B-X]**	Frequency of B - X at topological distance 4	2D Atom Pairs
4401	**F04[Si-Si]**	Frequency of Si - Si at topological distance 4	2D Atom Pairs
4402	**F04[Si-X]**	Frequency of Si - X at topological distance 4	2D Atom Pairs
4403	**F04[X-X]**	Frequency of X - X at topological distance 4	2D Atom Pairs
4404	**F05[C-C]**	Frequency of C - C at topological distance 5	2D Atom Pairs
4405	**F05[C-N]**	Frequency of C - N at topological distance 5	2D Atom Pairs
4406	**F05[C-O]**	Frequency of C - O at topological distance 5	2D Atom Pairs

No.	Name	Description	Block
4407	**F05[C-S]**	Frequency of C - S at topological distance 5	2D Atom Pairs
4408	**F05[C-P]**	Frequency of C - P at topological distance 5	2D Atom Pairs
4409	**F05[C-F]**	Frequency of C - F at topological distance 5	2D Atom Pairs
4410	**F05[C-Cl]**	Frequency of C - Cl at topological distance 5	2D Atom Pairs
4411	**F05[C-Br]**	Frequency of C - Br at topological distance 5	2D Atom Pairs
4412	**F05[C-I]**	Frequency of C - I at topological distance 5	2D Atom Pairs
4413	**F05[C-B]**	Frequency of C - B at topological distance 5	2D Atom Pairs
4414	**F05[C-Si]**	Frequency of C - Si at topological distance 5	2D Atom Pairs
4415	**F05[C-X]**	Frequency of C - X at topological distance 5	2D Atom Pairs
4416	**F05[N-N]**	Frequency of N - N at topological distance 5	2D Atom Pairs
4417	**F05[N-O]**	Frequency of N - O at topological distance 5	2D Atom Pairs
4418	**F05[N-S]**	Frequency of N - S at topological distance 5	2D Atom Pairs
4419	**F05[N-P]**	Frequency of N - P at topological distance 5	2D Atom Pairs
4420	**F05[N-F]**	Frequency of N - F at topological distance 5	2D Atom Pairs
4421	**F05[N-Cl]**	Frequency of N - Cl at topological distance 5	2D Atom Pairs
4422	**F05[N-Br]**	Frequency of N - Br at topological distance 5	2D Atom Pairs
4423	**F05[N-I]**	Frequency of N - I at topological distance 5	2D Atom Pairs
4424	**F05[N-B]**	Frequency of N - B at topological distance 5	2D Atom Pairs
4425	**F05[N-Si]**	Frequency of N - Si at topological distance 5	2D Atom Pairs
4426	**F05[N-X]**	Frequency of N - X at topological distance 5	2D Atom Pairs
4427	**F05[O-O]**	Frequency of O - O at topological distance 5	2D Atom Pairs
4428	**F05[O-S]**	Frequency of O - S at topological distance 5	2D Atom Pairs
4429	**F05[O-P]**	Frequency of O - P at topological distance 5	2D Atom Pairs
4430	**F05[O-F]**	Frequency of O - F at topological distance 5	2D Atom Pairs
4431	**F05[O-Cl]**	Frequency of O - Cl at topological distance 5	2D Atom Pairs
4432	**F05[O-Br]**	Frequency of O - Br at topological distance 5	2D Atom Pairs
4433	**F05[O-I]**	Frequency of O - I at topological distance 5	2D Atom Pairs
4434	**F05[O-B]**	Frequency of O - B at topological distance 5	2D Atom Pairs
4435	**F05[O-Si]**	Frequency of O - Si at topological distance 5	2D Atom Pairs
4436	**F05[O-X]**	Frequency of O - X at topological distance 5	2D Atom Pairs
4437	**F05[S-S]**	Frequency of S - S at topological distance 5	2D Atom Pairs
4438	**F05[S-P]**	Frequency of S - P at topological distance 5	2D Atom Pairs

No.	Name	Description	Block
4439	**F05[S-F]**	Frequency of S - F at topological distance 5	2D Atom Pairs
4440	**F05[S-Cl]**	Frequency of S - Cl at topological distance 5	2D Atom Pairs
4441	**F05[S-Br]**	Frequency of S - Br at topological distance 5	2D Atom Pairs
4442	**F05[S-I]**	Frequency of S - I at topological distance 5	2D Atom Pairs
4443	**F05[S-B]**	Frequency of S - B at topological distance 5	2D Atom Pairs
4444	**F05[S-Si]**	Frequency of S - Si at topological distance 5	2D Atom Pairs
4445	**F05[S-X]**	Frequency of S - X at topological distance 5	2D Atom Pairs
4446	**F05[P-P]**	Frequency of P - P at topological distance 5	2D Atom Pairs
4447	**F05[P-F]**	Frequency of P - F at topological distance 5	2D Atom Pairs
4448	**F05[P-Cl]**	Frequency of P - Cl at topological distance 5	2D Atom Pairs
4449	**F05[P-Br]**	Frequency of P - Br at topological distance 5	2D Atom Pairs
4450	**F05[P-I]**	Frequency of P - I at topological distance 5	2D Atom Pairs
4451	**F05[P-B]**	Frequency of P - B at topological distance 5	2D Atom Pairs
4452	**F05[P-Si]**	Frequency of P - Si at topological distance 5	2D Atom Pairs
4453	**F05[P-X]**	Frequency of P - X at topological distance 5	2D Atom Pairs
4454	**F05[F-F]**	Frequency of F - F at topological distance 5	2D Atom Pairs
4455	**F05[F-Cl]**	Frequency of F - Cl at topological distance 5	2D Atom Pairs
4456	**F05[F-Br]**	Frequency of F - Br at topological distance 5	2D Atom Pairs
4457	**F05[F-I]**	Frequency of F - I at topological distance 5	2D Atom Pairs
4458	**F05[F-B]**	Frequency of F - B at topological distance 5	2D Atom Pairs
4459	**F05[F-Si]**	Frequency of F - Si at topological distance 5	2D Atom Pairs
4460	**F05[F-X]**	Frequency of F - X at topological distance 5	2D Atom Pairs
4461	**F05[Cl-Cl]**	Frequency of Cl - Cl at topological distance 5	2D Atom Pairs
4462	**F05[Cl-Br]**	Frequency of Cl - Br at topological distance 5	2D Atom Pairs
4463	**F05[Cl-I]**	Frequency of Cl - I at topological distance 5	2D Atom Pairs
4464	**F05[Cl-B]**	Frequency of Cl - B at topological distance 5	2D Atom Pairs
4465	**F05[Cl-Si]**	Frequency of Cl - Si at topological distance 5	2D Atom Pairs
4466	**F05[Cl-X]**	Frequency of Cl - X at topological distance 5	2D Atom Pairs
4467	**F05[Br-Br]**	Frequency of Br - Br at topological distance 5	2D Atom Pairs
4468	**F05[Br-I]**	Frequency of Br - I at topological distance 5	2D Atom Pairs
4469	**F05[Br-B]**	Frequency of Br - B at topological distance 5	2D Atom Pairs
4470	**F05[Br-Si]**	Frequency of Br - Si at topological distance 5	2D Atom Pairs

No.	Name	Description	Block
4471	**F05[Br-X]**	Frequency of Br - X at topological distance 5	2D Atom Pairs
4472	**F05[I-I]**	Frequency of I - I at topological distance 5	2D Atom Pairs
4473	**F05[I-B]**	Frequency of I - B at topological distance 5	2D Atom Pairs
4474	**F05[I-Si]**	Frequency of I - Si at topological distance 5	2D Atom Pairs
4475	**F05[I-X]**	Frequency of I - X at topological distance 5	2D Atom Pairs
4476	**F05[B-B]**	Frequency of B - B at topological distance 5	2D Atom Pairs
4477	**F05[B-Si]**	Frequency of B - Si at topological distance 5	2D Atom Pairs
4478	**F05[B-X]**	Frequency of B - X at topological distance 5	2D Atom Pairs
4479	**F05[Si-Si]**	Frequency of Si - Si at topological distance 5	2D Atom Pairs
4480	**F05[Si-X]**	Frequency of Si - X at topological distance 5	2D Atom Pairs
4481	**F05[X-X]**	Frequency of X - X at topological distance 5	2D Atom Pairs
4482	**F06[C-C]**	Frequency of C - C at topological distance 6	2D Atom Pairs
4483	**F06[C-N]**	Frequency of C - N at topological distance 6	2D Atom Pairs
4484	**F06[C-O]**	Frequency of C - O at topological distance 6	2D Atom Pairs
4485	**F06[C-S]**	Frequency of C - S at topological distance 6	2D Atom Pairs
4486	**F06[C-P]**	Frequency of C - P at topological distance 6	2D Atom Pairs
4487	**F06[C-F]**	Frequency of C - F at topological distance 6	2D Atom Pairs
4488	**F06[C-Cl]**	Frequency of C - Cl at topological distance 6	2D Atom Pairs
4489	**F06[C-Br]**	Frequency of C - Br at topological distance 6	2D Atom Pairs
4490	**F06[C-I]**	Frequency of C - I at topological distance 6	2D Atom Pairs
4491	**F06[C-B]**	Frequency of C - B at topological distance 6	2D Atom Pairs
4492	**F06[C-Si]**	Frequency of C - Si at topological distance 6	2D Atom Pairs
4493	**F06[C-X]**	Frequency of C - X at topological distance 6	2D Atom Pairs
4494	**F06[N-N]**	Frequency of N - N at topological distance 6	2D Atom Pairs
4495	**F06[N-O]**	Frequency of N - O at topological distance 6	2D Atom Pairs
4496	**F06[N-S]**	Frequency of N - S at topological distance 6	2D Atom Pairs
4497	**F06[N-P]**	Frequency of N - P at topological distance 6	2D Atom Pairs
4498	**F06[N-F]**	Frequency of N - F at topological distance 6	2D Atom Pairs
4499	**F06[N-Cl]**	Frequency of N - Cl at topological distance 6	2D Atom Pairs
4500	**F06[N-Br]**	Frequency of N - Br at topological distance 6	2D Atom Pairs
4501	**F06[N-I]**	Frequency of N - I at topological distance 6	2D Atom Pairs
4502	**F06[N-B]**	Frequency of N - B at topological distance 6	2D Atom Pairs

No.	Name	Description	Block
4503	**F06[N-Si]**	Frequency of N - Si at topological distance 6	2D Atom Pairs
4504	**F06[N-X]**	Frequency of N - X at topological distance 6	2D Atom Pairs
4505	**F06[O-O]**	Frequency of O - O at topological distance 6	2D Atom Pairs
4506	**F06[O-S]**	Frequency of O - S at topological distance 6	2D Atom Pairs
4507	**F06[O-P]**	Frequency of O - P at topological distance 6	2D Atom Pairs
4508	**F06[O-F]**	Frequency of O - F at topological distance 6	2D Atom Pairs
4509	**F06[O-Cl]**	Frequency of O - Cl at topological distance 6	2D Atom Pairs
4510	**F06[O-Br]**	Frequency of O - Br at topological distance 6	2D Atom Pairs
4511	**F06[O-I]**	Frequency of O - I at topological distance 6	2D Atom Pairs
4512	**F06[O-B]**	Frequency of O - B at topological distance 6	2D Atom Pairs
4513	**F06[O-Si]**	Frequency of O - Si at topological distance 6	2D Atom Pairs
4514	**F06[O-X]**	Frequency of O - X at topological distance 6	2D Atom Pairs
4515	**F06[S-S]**	Frequency of S - S at topological distance 6	2D Atom Pairs
4516	**F06[S-P]**	Frequency of S - P at topological distance 6	2D Atom Pairs
4517	**F06[S-F]**	Frequency of S - F at topological distance 6	2D Atom Pairs
4518	**F06[S-Cl]**	Frequency of S - Cl at topological distance 6	2D Atom Pairs
4519	**F06[S-Br]**	Frequency of S - Br at topological distance 6	2D Atom Pairs
4520	**F06[S-I]**	Frequency of S - I at topological distance 6	2D Atom Pairs
4521	**F06[S-B]**	Frequency of S - B at topological distance 6	2D Atom Pairs
4522	**F06[S-Si]**	Frequency of S - Si at topological distance 6	2D Atom Pairs
4523	**F06[S-X]**	Frequency of S - X at topological distance 6	2D Atom Pairs
4524	**F06[P-P]**	Frequency of P - P at topological distance 6	2D Atom Pairs
4525	**F06[P-F]**	Frequency of P - F at topological distance 6	2D Atom Pairs
4526	**F06[P-Cl]**	Frequency of P - Cl at topological distance 6	2D Atom Pairs
4527	**F06[P-Br]**	Frequency of P - Br at topological distance 6	2D Atom Pairs
4528	**F06[P-I]**	Frequency of P - I at topological distance 6	2D Atom Pairs
4529	**F06[P-B]**	Frequency of P - B at topological distance 6	2D Atom Pairs
4530	**F06[P-Si]**	Frequency of P - Si at topological distance 6	2D Atom Pairs
4531	**F06[P-X]**	Frequency of P - X at topological distance 6	2D Atom Pairs
4532	**F06[F-F]**	Frequency of F - F at topological distance 6	2D Atom Pairs
4533	**F06[F-Cl]**	Frequency of F - Cl at topological distance 6	2D Atom Pairs
4534	**F06[F-Br]**	Frequency of F - Br at topological distance 6	2D Atom Pairs

No.	Name	Description	Block
4535	**F06[F-I]**	Frequency of F - I at topological distance 6	2D Atom Pairs
4536	**F06[F-B]**	Frequency of F - B at topological distance 6	2D Atom Pairs
4537	**F06[F-Si]**	Frequency of F - Si at topological distance 6	2D Atom Pairs
4538	**F06[F-X]**	Frequency of F - X at topological distance 6	2D Atom Pairs
4539	**F06[Cl-Cl]**	Frequency of Cl - Cl at topological distance 6	2D Atom Pairs
4540	**F06[Cl-Br]**	Frequency of Cl - Br at topological distance 6	2D Atom Pairs
4541	**F06[Cl-I]**	Frequency of Cl - I at topological distance 6	2D Atom Pairs
4542	**F06[Cl-B]**	Frequency of Cl - B at topological distance 6	2D Atom Pairs
4543	**F06[Cl-Si]**	Frequency of Cl - Si at topological distance 6	2D Atom Pairs
4544	**F06[Cl-X]**	Frequency of Cl - X at topological distance 6	2D Atom Pairs
4545	**F06[Br-Br]**	Frequency of Br - Br at topological distance 6	2D Atom Pairs
4546	**F06[Br-I]**	Frequency of Br - I at topological distance 6	2D Atom Pairs
4547	**F06[Br-B]**	Frequency of Br - B at topological distance 6	2D Atom Pairs
4548	**F06[Br-Si]**	Frequency of Br - Si at topological distance 6	2D Atom Pairs
4549	**F06[Br-X]**	Frequency of Br - X at topological distance 6	2D Atom Pairs
4550	**F06[I-I]**	Frequency of I - I at topological distance 6	2D Atom Pairs
4551	**F06[I-B]**	Frequency of I - B at topological distance 6	2D Atom Pairs
4552	**F06[I-Si]**	Frequency of I - Si at topological distance 6	2D Atom Pairs
4553	**F06[I-X]**	Frequency of I - X at topological distance 6	2D Atom Pairs
4554	**F06[B-B]**	Frequency of B - B at topological distance 6	2D Atom Pairs
4555	**F06[B-Si]**	Frequency of B - Si at topological distance 6	2D Atom Pairs
4556	**F06[B-X]**	Frequency of B - X at topological distance 6	2D Atom Pairs
4557	**F06[Si-Si]**	Frequency of Si - Si at topological distance 6	2D Atom Pairs
4558	**F06[Si-X]**	Frequency of Si - X at topological distance 6	2D Atom Pairs
4559	**F06[X-X]**	Frequency of X - X at topological distance 6	2D Atom Pairs
4560	**F07[C-C]**	Frequency of C - C at topological distance 7	2D Atom Pairs
4561	**F07[C-N]**	Frequency of C - N at topological distance 7	2D Atom Pairs
4562	**F07[C-O]**	Frequency of C - O at topological distance 7	2D Atom Pairs
4563	**F07[C-S]**	Frequency of C - S at topological distance 7	2D Atom Pairs
4564	**F07[C-P]**	Frequency of C - P at topological distance 7	2D Atom Pairs
4565	**F07[C-F]**	Frequency of C - F at topological distance 7	2D Atom Pairs
4566	**F07[C-Cl]**	Frequency of C - Cl at topological distance 7	2D Atom Pairs

No.	Name	Description	Block
4567	**F07[C-Br]**	Frequency of C - Br at topological distance 7	2D Atom Pairs
4568	**F07[C-I]**	Frequency of C - I at topological distance 7	2D Atom Pairs
4569	**F07[C-B]**	Frequency of C - B at topological distance 7	2D Atom Pairs
4570	**F07[C-Si]**	Frequency of C - Si at topological distance 7	2D Atom Pairs
4571	**F07[C-X]**	Frequency of C - X at topological distance 7	2D Atom Pairs
4572	**F07[N-N]**	Frequency of N - N at topological distance 7	2D Atom Pairs
4573	**F07[N-O]**	Frequency of N - O at topological distance 7	2D Atom Pairs
4574	**F07[N-S]**	Frequency of N - S at topological distance 7	2D Atom Pairs
4575	**F07[N-P]**	Frequency of N - P at topological distance 7	2D Atom Pairs
4576	**F07[N-F]**	Frequency of N - F at topological distance 7	2D Atom Pairs
4577	**F07[N-Cl]**	Frequency of N - Cl at topological distance 7	2D Atom Pairs
4578	**F07[N-Br]**	Frequency of N - Br at topological distance 7	2D Atom Pairs
4579	**F07[N-I]**	Frequency of N - I at topological distance 7	2D Atom Pairs
4580	**F07[N-B]**	Frequency of N - B at topological distance 7	2D Atom Pairs
4581	**F07[N-Si]**	Frequency of N - Si at topological distance 7	2D Atom Pairs
4582	**F07[N-X]**	Frequency of N - X at topological distance 7	2D Atom Pairs
4583	**F07[O-O]**	Frequency of O - O at topological distance 7	2D Atom Pairs
4584	**F07[O-S]**	Frequency of O - S at topological distance 7	2D Atom Pairs
4585	**F07[O-P]**	Frequency of O - P at topological distance 7	2D Atom Pairs
4586	**F07[O-F]**	Frequency of O - F at topological distance 7	2D Atom Pairs
4587	**F07[O-Cl]**	Frequency of O - Cl at topological distance 7	2D Atom Pairs
4588	**F07[O-Br]**	Frequency of O - Br at topological distance 7	2D Atom Pairs
4589	**F07[O-I]**	Frequency of O - I at topological distance 7	2D Atom Pairs
4590	**F07[O-B]**	Frequency of O - B at topological distance 7	2D Atom Pairs
4591	**F07[O-Si]**	Frequency of O - Si at topological distance 7	2D Atom Pairs
4592	**F07[O-X]**	Frequency of O - X at topological distance 7	2D Atom Pairs
4593	**F07[S-S]**	Frequency of S - S at topological distance 7	2D Atom Pairs
4594	**F07[S-P]**	Frequency of S - P at topological distance 7	2D Atom Pairs
4595	**F07[S-F]**	Frequency of S - F at topological distance 7	2D Atom Pairs
4596	**F07[S-Cl]**	Frequency of S - Cl at topological distance 7	2D Atom Pairs
4597	**F07[S-Br]**	Frequency of S - Br at topological distance 7	2D Atom Pairs
4598	**F07[S-I]**	Frequency of S - I at topological distance 7	2D Atom Pairs

No.	Name	Description	Block
4599	**F07[S-B]**	Frequency of S - B at topological distance 7	2D Atom Pairs
4600	**F07[S-Si]**	Frequency of S - Si at topological distance 7	2D Atom Pairs
4601	**F07[S-X]**	Frequency of S - X at topological distance 7	2D Atom Pairs
4602	**F07[P-P]**	Frequency of P - P at topological distance 7	2D Atom Pairs
4603	**F07[P-F]**	Frequency of P - F at topological distance 7	2D Atom Pairs
4604	**F07[P-Cl]**	Frequency of P - Cl at topological distance 7	2D Atom Pairs
4605	**F07[P-Br]**	Frequency of P - Br at topological distance 7	2D Atom Pairs
4606	**F07[P-I]**	Frequency of P - I at topological distance 7	2D Atom Pairs
4607	**F07[P-B]**	Frequency of P - B at topological distance 7	2D Atom Pairs
4608	**F07[P-Si]**	Frequency of P - Si at topological distance 7	2D Atom Pairs
4609	**F07[P-X]**	Frequency of P - X at topological distance 7	2D Atom Pairs
4610	**F07[F-F]**	Frequency of F - F at topological distance 7	2D Atom Pairs
4611	**F07[F-Cl]**	Frequency of F - Cl at topological distance 7	2D Atom Pairs
4612	**F07[F-Br]**	Frequency of F - Br at topological distance 7	2D Atom Pairs
4613	**F07[F-I]**	Frequency of F - I at topological distance 7	2D Atom Pairs
4614	**F07[F-B]**	Frequency of F - B at topological distance 7	2D Atom Pairs
4615	**F07[F-Si]**	Frequency of F - Si at topological distance 7	2D Atom Pairs
4616	**F07[F-X]**	Frequency of F - X at topological distance 7	2D Atom Pairs
4617	**F07[Cl-Cl]**	Frequency of Cl - Cl at topological distance 7	2D Atom Pairs
4618	**F07[Cl-Br]**	Frequency of Cl - Br at topological distance 7	2D Atom Pairs
4619	**F07[Cl-I]**	Frequency of Cl - I at topological distance 7	2D Atom Pairs
4620	**F07[Cl-B]**	Frequency of Cl - B at topological distance 7	2D Atom Pairs
4621	**F07[Cl-Si]**	Frequency of Cl - Si at topological distance 7	2D Atom Pairs
4622	**F07[Cl-X]**	Frequency of Cl - X at topological distance 7	2D Atom Pairs
4623	**F07[Br-Br]**	Frequency of Br - Br at topological distance 7	2D Atom Pairs
4624	**F07[Br-I]**	Frequency of Br - I at topological distance 7	2D Atom Pairs
4625	**F07[Br-B]**	Frequency of Br - B at topological distance 7	2D Atom Pairs
4626	**F07[Br-Si]**	Frequency of Br - Si at topological distance 7	2D Atom Pairs
4627	**F07[Br-X]**	Frequency of Br - X at topological distance 7	2D Atom Pairs
4628	**F07[I-I]**	Frequency of I - I at topological distance 7	2D Atom Pairs
4629	**F07[I-B]**	Frequency of I - B at topological distance 7	2D Atom Pairs
4630	**F07[I-Si]**	Frequency of I - Si at topological distance 7	2D Atom Pairs

No.	Name	Description	Block
4631	**F07[I-X]**	Frequency of I - X at topological distance 7	2D Atom Pairs
4632	**F07[B-B]**	Frequency of B - B at topological distance 7	2D Atom Pairs
4633	**F07[B-Si]**	Frequency of B - Si at topological distance 7	2D Atom Pairs
4634	**F07[B-X]**	Frequency of B - X at topological distance 7	2D Atom Pairs
4635	**F07[Si-Si]**	Frequency of Si - Si at topological distance 7	2D Atom Pairs
4636	**F07[Si-X]**	Frequency of Si - X at topological distance 7	2D Atom Pairs
4637	**F07[X-X]**	Frequency of X - X at topological distance 7	2D Atom Pairs
4638	**F08[C-C]**	Frequency of C - C at topological distance 8	2D Atom Pairs
4639	**F08[C-N]**	Frequency of C - N at topological distance 8	2D Atom Pairs
4640	**F08[C-O]**	Frequency of C - O at topological distance 8	2D Atom Pairs
4641	**F08[C-S]**	Frequency of C - S at topological distance 8	2D Atom Pairs
4642	**F08[C-P]**	Frequency of C - P at topological distance 8	2D Atom Pairs
4643	**F08[C-F]**	Frequency of C - F at topological distance 8	2D Atom Pairs
4644	**F08[C-Cl]**	Frequency of C - Cl at topological distance 8	2D Atom Pairs
4645	**F08[C-Br]**	Frequency of C - Br at topological distance 8	2D Atom Pairs
4646	**F08[C-I]**	Frequency of C - I at topological distance 8	2D Atom Pairs
4647	**F08[C-B]**	Frequency of C - B at topological distance 8	2D Atom Pairs
4648	**F08[C-Si]**	Frequency of C - Si at topological distance 8	2D Atom Pairs
4649	**F08[C-X]**	Frequency of C - X at topological distance 8	2D Atom Pairs
4650	**F08[N-N]**	Frequency of N - N at topological distance 8	2D Atom Pairs
4651	**F08[N-O]**	Frequency of N - O at topological distance 8	2D Atom Pairs
4652	**F08[N-S]**	Frequency of N - S at topological distance 8	2D Atom Pairs
4653	**F08[N-P]**	Frequency of N - P at topological distance 8	2D Atom Pairs
4654	**F08[N-F]**	Frequency of N - F at topological distance 8	2D Atom Pairs
4655	**F08[N-Cl]**	Frequency of N - Cl at topological distance 8	2D Atom Pairs
4656	**F08[N-Br]**	Frequency of N - Br at topological distance 8	2D Atom Pairs
4657	**F08[N-I]**	Frequency of N - I at topological distance 8	2D Atom Pairs
4658	**F08[N-B]**	Frequency of N - B at topological distance 8	2D Atom Pairs
4659	**F08[N-Si]**	Frequency of N - Si at topological distance 8	2D Atom Pairs
4660	**F08[N-X]**	Frequency of N - X at topological distance 8	2D Atom Pairs
4661	**F08[O-O]**	Frequency of O - O at topological distance 8	2D Atom Pairs
4662	**F08[O-S]**	Frequency of O - S at topological distance 8	2D Atom Pairs

No.	Name	Description	Block
4663	**F08[O-P]**	Frequency of O - P at topological distance 8	2D Atom Pairs
4664	**F08[O-F]**	Frequency of O - F at topological distance 8	2D Atom Pairs
4665	**F08[O-Cl]**	Frequency of O - Cl at topological distance 8	2D Atom Pairs
4666	**F08[O-Br]**	Frequency of O - Br at topological distance 8	2D Atom Pairs
4667	**F08[O-I]**	Frequency of O - I at topological distance 8	2D Atom Pairs
4668	**F08[O-B]**	Frequency of O - B at topological distance 8	2D Atom Pairs
4669	**F08[O-Si]**	Frequency of O - Si at topological distance 8	2D Atom Pairs
4670	**F08[O-X]**	Frequency of O - X at topological distance 8	2D Atom Pairs
4671	**F08[S-S]**	Frequency of S - S at topological distance 8	2D Atom Pairs
4672	**F08[S-P]**	Frequency of S - P at topological distance 8	2D Atom Pairs
4673	**F08[S-F]**	Frequency of S - F at topological distance 8	2D Atom Pairs
4674	**F08[S-Cl]**	Frequency of S - Cl at topological distance 8	2D Atom Pairs
4675	**F08[S-Br]**	Frequency of S - Br at topological distance 8	2D Atom Pairs
4676	**F08[S-I]**	Frequency of S - I at topological distance 8	2D Atom Pairs
4677	**F08[S-B]**	Frequency of S - B at topological distance 8	2D Atom Pairs
4678	**F08[S-Si]**	Frequency of S - Si at topological distance 8	2D Atom Pairs
4679	**F08[S-X]**	Frequency of S - X at topological distance 8	2D Atom Pairs
4680	**F08[P-P]**	Frequency of P - P at topological distance 8	2D Atom Pairs
4681	**F08[P-F]**	Frequency of P - F at topological distance 8	2D Atom Pairs
4682	**F08[P-Cl]**	Frequency of P - Cl at topological distance 8	2D Atom Pairs
4683	**F08[P-Br]**	Frequency of P - Br at topological distance 8	2D Atom Pairs
4684	**F08[P-I]**	Frequency of P - I at topological distance 8	2D Atom Pairs
4685	**F08[P-B]**	Frequency of P - B at topological distance 8	2D Atom Pairs
4686	**F08[P-Si]**	Frequency of P - Si at topological distance 8	2D Atom Pairs
4687	**F08[P-X]**	Frequency of P - X at topological distance 8	2D Atom Pairs
4688	**F08[F-F]**	Frequency of F - F at topological distance 8	2D Atom Pairs
4689	**F08[F-Cl]**	Frequency of F - Cl at topological distance 8	2D Atom Pairs
4690	**F08[F-Br]**	Frequency of F - Br at topological distance 8	2D Atom Pairs
4691	**F08[F-I]**	Frequency of F - I at topological distance 8	2D Atom Pairs
4692	**F08[F-B]**	Frequency of F - B at topological distance 8	2D Atom Pairs
4693	**F08[F-Si]**	Frequency of F - Si at topological distance 8	2D Atom Pairs
4694	**F08[F-X]**	Frequency of F - X at topological distance 8	2D Atom Pairs

No.	Name	Description	Block
4695	**F08[Cl-Cl]**	Frequency of Cl - Cl at topological distance 8	2D Atom Pairs
4696	**F08[Cl-Br]**	Frequency of Cl - Br at topological distance 8	2D Atom Pairs
4697	**F08[Cl-I]**	Frequency of Cl - I at topological distance 8	2D Atom Pairs
4698	**F08[Cl-B]**	Frequency of Cl - B at topological distance 8	2D Atom Pairs
4699	**F08[Cl-Si]**	Frequency of Cl - Si at topological distance 8	2D Atom Pairs
4700	**F08[Cl-X]**	Frequency of Cl - X at topological distance 8	2D Atom Pairs
4701	**F08[Br-Br]**	Frequency of Br - Br at topological distance 8	2D Atom Pairs
4702	**F08[Br-I]**	Frequency of Br - I at topological distance 8	2D Atom Pairs
4703	**F08[Br-B]**	Frequency of Br - B at topological distance 8	2D Atom Pairs
4704	**F08[Br-Si]**	Frequency of Br - Si at topological distance 8	2D Atom Pairs
4705	**F08[Br-X]**	Frequency of Br - X at topological distance 8	2D Atom Pairs
4706	**F08[I-I]**	Frequency of I - I at topological distance 8	2D Atom Pairs
4707	**F08[I-B]**	Frequency of I - B at topological distance 8	2D Atom Pairs
4708	**F08[I-Si]**	Frequency of I - Si at topological distance 8	2D Atom Pairs
4709	**F08[I-X]**	Frequency of I - X at topological distance 8	2D Atom Pairs
4710	**F08[B-B]**	Frequency of B - B at topological distance 8	2D Atom Pairs
4711	**F08[B-Si]**	Frequency of B - Si at topological distance 8	2D Atom Pairs
4712	**F08[B-X]**	Frequency of B - X at topological distance 8	2D Atom Pairs
4713	**F08[Si-Si]**	Frequency of Si - Si at topological distance 8	2D Atom Pairs
4714	**F08[Si-X]**	Frequency of Si - X at topological distance 8	2D Atom Pairs
4715	**F08[X-X]**	Frequency of X - X at topological distance 8	2D Atom Pairs
4716	**F09[C-C]**	Frequency of C - C at topological distance 9	2D Atom Pairs
4717	**F09[C-N]**	Frequency of C - N at topological distance 9	2D Atom Pairs
4718	**F09[C-O]**	Frequency of C - O at topological distance 9	2D Atom Pairs
4719	**F09[C-S]**	Frequency of C - S at topological distance 9	2D Atom Pairs
4720	**F09[C-P]**	Frequency of C - P at topological distance 9	2D Atom Pairs
4721	**F09[C-F]**	Frequency of C - F at topological distance 9	2D Atom Pairs
4722	**F09[C-Cl]**	Frequency of C - Cl at topological distance 9	2D Atom Pairs
4723	**F09[C-Br]**	Frequency of C - Br at topological distance 9	2D Atom Pairs
4724	**F09[C-I]**	Frequency of C - I at topological distance 9	2D Atom Pairs
4725	**F09[C-B]**	Frequency of C - B at topological distance 9	2D Atom Pairs
4726	**F09[C-Si]**	Frequency of C - Si at topological distance 9	2D Atom Pairs

No.	Name	Description	Block
4727	**F09[C-X]**	Frequency of C - X at topological distance 9	2D Atom Pairs
4728	**F09[N-N]**	Frequency of N - N at topological distance 9	2D Atom Pairs
4729	**F09[N-O]**	Frequency of N - O at topological distance 9	2D Atom Pairs
4730	**F09[N-S]**	Frequency of N - S at topological distance 9	2D Atom Pairs
4731	**F09[N-P]**	Frequency of N - P at topological distance 9	2D Atom Pairs
4732	**F09[N-F]**	Frequency of N - F at topological distance 9	2D Atom Pairs
4733	**F09[N-Cl]**	Frequency of N - Cl at topological distance 9	2D Atom Pairs
4734	**F09[N-Br]**	Frequency of N - Br at topological distance 9	2D Atom Pairs
4735	**F09[N-I]**	Frequency of N - I at topological distance 9	2D Atom Pairs
4736	**F09[N-B]**	Frequency of N - B at topological distance 9	2D Atom Pairs
4737	**F09[N-Si]**	Frequency of N - Si at topological distance 9	2D Atom Pairs
4738	**F09[N-X]**	Frequency of N - X at topological distance 9	2D Atom Pairs
4739	**F09[O-O]**	Frequency of O - O at topological distance 9	2D Atom Pairs
4740	**F09[O-S]**	Frequency of O - S at topological distance 9	2D Atom Pairs
4741	**F09[O-P]**	Frequency of O - P at topological distance 9	2D Atom Pairs
4742	**F09[O-F]**	Frequency of O - F at topological distance 9	2D Atom Pairs
4743	**F09[O-Cl]**	Frequency of O - Cl at topological distance 9	2D Atom Pairs
4744	**F09[O-Br]**	Frequency of O - Br at topological distance 9	2D Atom Pairs
4745	**F09[O-I]**	Frequency of O - I at topological distance 9	2D Atom Pairs
4746	**F09[O-B]**	Frequency of O - B at topological distance 9	2D Atom Pairs
4747	**F09[O-Si]**	Frequency of O - Si at topological distance 9	2D Atom Pairs
4748	**F09[O-X]**	Frequency of O - X at topological distance 9	2D Atom Pairs
4749	**F09[S-S]**	Frequency of S - S at topological distance 9	2D Atom Pairs
4750	**F09[S-P]**	Frequency of S - P at topological distance 9	2D Atom Pairs
4751	**F09[S-F]**	Frequency of S - F at topological distance 9	2D Atom Pairs
4752	**F09[S-Cl]**	Frequency of S - Cl at topological distance 9	2D Atom Pairs
4753	**F09[S-Br]**	Frequency of S - Br at topological distance 9	2D Atom Pairs
4754	**F09[S-I]**	Frequency of S - I at topological distance 9	2D Atom Pairs
4755	**F09[S-B]**	Frequency of S - B at topological distance 9	2D Atom Pairs
4756	**F09[S-Si]**	Frequency of S - Si at topological distance 9	2D Atom Pairs
4757	**F09[S-X]**	Frequency of S - X at topological distance 9	2D Atom Pairs
4758	**F09[P-P]**	Frequency of P - P at topological distance 9	2D Atom Pairs

No.	Name	Description	Block
4759	**F09[P-F]**	Frequency of P - F at topological distance 9	2D Atom Pairs
4760	**F09[P-Cl]**	Frequency of P - Cl at topological distance 9	2D Atom Pairs
4761	**F09[P-Br]**	Frequency of P - Br at topological distance 9	2D Atom Pairs
4762	**F09[P-I]**	Frequency of P - I at topological distance 9	2D Atom Pairs
4763	**F09[P-B]**	Frequency of P - B at topological distance 9	2D Atom Pairs
4764	**F09[P-Si]**	Frequency of P - Si at topological distance 9	2D Atom Pairs
4765	**F09[P-X]**	Frequency of P - X at topological distance 9	2D Atom Pairs
4766	**F09[F-F]**	Frequency of F - F at topological distance 9	2D Atom Pairs
4767	**F09[F-Cl]**	Frequency of F - Cl at topological distance 9	2D Atom Pairs
4768	**F09[F-Br]**	Frequency of F - Br at topological distance 9	2D Atom Pairs
4769	**F09[F-I]**	Frequency of F - I at topological distance 9	2D Atom Pairs
4770	**F09[F-B]**	Frequency of F - B at topological distance 9	2D Atom Pairs
4771	**F09[F-Si]**	Frequency of F - Si at topological distance 9	2D Atom Pairs
4772	**F09[F-X]**	Frequency of F - X at topological distance 9	2D Atom Pairs
4773	**F09[Cl-Cl]**	Frequency of Cl - Cl at topological distance 9	2D Atom Pairs
4774	**F09[Cl-Br]**	Frequency of Cl - Br at topological distance 9	2D Atom Pairs
4775	**F09[Cl-I]**	Frequency of Cl - I at topological distance 9	2D Atom Pairs
4776	**F09[Cl-B]**	Frequency of Cl - B at topological distance 9	2D Atom Pairs
4777	**F09[Cl-Si]**	Frequency of Cl - Si at topological distance 9	2D Atom Pairs
4778	**F09[Cl-X]**	Frequency of Cl - X at topological distance 9	2D Atom Pairs
4779	**F09[Br-Br]**	Frequency of Br - Br at topological distance 9	2D Atom Pairs
4780	**F09[Br-I]**	Frequency of Br - I at topological distance 9	2D Atom Pairs
4781	**F09[Br-B]**	Frequency of Br - B at topological distance 9	2D Atom Pairs
4782	**F09[Br-Si]**	Frequency of Br - Si at topological distance 9	2D Atom Pairs
4783	**F09[Br-X]**	Frequency of Br - X at topological distance 9	2D Atom Pairs
4784	**F09[I-I]**	Frequency of I - I at topological distance 9	2D Atom Pairs
4785	**F09[I-B]**	Frequency of I - B at topological distance 9	2D Atom Pairs
4786	**F09[I-Si]**	Frequency of I - Si at topological distance 9	2D Atom Pairs
4787	**F09[I-X]**	Frequency of I - X at topological distance 9	2D Atom Pairs
4788	**F09[B-B]**	Frequency of B - B at topological distance 9	2D Atom Pairs
4789	**F09[B-Si]**	Frequency of B - Si at topological distance 9	2D Atom Pairs
4790	**F09[B-X]**	Frequency of B - X at topological distance 9	2D Atom Pairs

No.	Name	Description	Block
4791	**F09[Si-Si]**	Frequency of Si - Si at topological distance 9	2D Atom Pairs
4792	**F09[Si-X]**	Frequency of Si - X at topological distance 9	2D Atom Pairs
4793	**F09[X-X]**	Frequency of X - X at topological distance 9	2D Atom Pairs
4794	**F10[C-C]**	Frequency of C - C at topological distance 10	2D Atom Pairs
4795	**F10[C-N]**	Frequency of C - N at topological distance 10	2D Atom Pairs
4796	**F10[C-O]**	Frequency of C - O at topological distance 10	2D Atom Pairs
4797	**F10[C-S]**	Frequency of C - S at topological distance 10	2D Atom Pairs
4798	**F10[C-P]**	Frequency of C - P at topological distance 10	2D Atom Pairs
4799	**F10[C-F]**	Frequency of C - F at topological distance 10	2D Atom Pairs
4800	**F10[C-Cl]**	Frequency of C - Cl at topological distance 10	2D Atom Pairs
4801	**F10[C-Br]**	Frequency of C - Br at topological distance 10	2D Atom Pairs
4802	**F10[C-I]**	Frequency of C - I at topological distance 10	2D Atom Pairs
4803	**F10[C-B]**	Frequency of C - B at topological distance 10	2D Atom Pairs
4804	**F10[C-Si]**	Frequency of C - Si at topological distance 10	2D Atom Pairs
4805	**F10[C-X]**	Frequency of C - X at topological distance 10	2D Atom Pairs
4806	**F10[N-N]**	Frequency of N - N at topological distance 10	2D Atom Pairs
4807	**F10[N-O]**	Frequency of N - O at topological distance 10	2D Atom Pairs
4808	**F10[N-S]**	Frequency of N - S at topological distance 10	2D Atom Pairs
4809	**F10[N-P]**	Frequency of N - P at topological distance 10	2D Atom Pairs
4810	**F10[N-F]**	Frequency of N - F at topological distance 10	2D Atom Pairs
4811	**F10[N-Cl]**	Frequency of N - Cl at topological distance 10	2D Atom Pairs
4812	**F10[N-Br]**	Frequency of N - Br at topological distance 10	2D Atom Pairs
4813	**F10[N-I]**	Frequency of N - I at topological distance 10	2D Atom Pairs
4814	**F10[N-B]**	Frequency of N - B at topological distance 10	2D Atom Pairs
4815	**F10[N-Si]**	Frequency of N - Si at topological distance 10	2D Atom Pairs
4816	**F10[N-X]**	Frequency of N - X at topological distance 10	2D Atom Pairs
4817	**F10[O-O]**	Frequency of O - O at topological distance 10	2D Atom Pairs
4818	**F10[O-S]**	Frequency of O - S at topological distance 10	2D Atom Pairs
4819	**F10[O-P]**	Frequency of O - P at topological distance 10	2D Atom Pairs
4820	**F10[O-F]**	Frequency of O - F at topological distance 10	2D Atom Pairs
4821	**F10[O-Cl]**	Frequency of O - Cl at topological distance 10	2D Atom Pairs
4822	**F10[O-Br]**	Frequency of O - Br at topological distance 10	2D Atom Pairs

No.	Name	Description	Block
4823	**F10[O-I]**	Frequency of O - I at topological distance 10	2D Atom Pairs
4824	**F10[O-B]**	Frequency of O - B at topological distance 10	2D Atom Pairs
4825	**F10[O-Si]**	Frequency of O - Si at topological distance 10	2D Atom Pairs
4826	**F10[O-X]**	Frequency of O - X at topological distance 10	2D Atom Pairs
4827	**F10[S-S]**	Frequency of S - S at topological distance 10	2D Atom Pairs
4828	**F10[S-P]**	Frequency of S - P at topological distance 10	2D Atom Pairs
4829	**F10[S-F]**	Frequency of S - F at topological distance 10	2D Atom Pairs
4830	**F10[S-Cl]**	Frequency of S - Cl at topological distance 10	2D Atom Pairs
4831	**F10[S-Br]**	Frequency of S - Br at topological distance 10	2D Atom Pairs
4832	**F10[S-I]**	Frequency of S - I at topological distance 10	2D Atom Pairs
4833	**F10[S-B]**	Frequency of S - B at topological distance 10	2D Atom Pairs
4834	**F10[S-Si]**	Frequency of S - Si at topological distance 10	2D Atom Pairs
4835	**F10[S-X]**	Frequency of S - X at topological distance 10	2D Atom Pairs
4836	**F10[P-P]**	Frequency of P - P at topological distance 10	2D Atom Pairs
4837	**F10[P-F]**	Frequency of P - F at topological distance 10	2D Atom Pairs
4838	**F10[P-Cl]**	Frequency of P - Cl at topological distance 10	2D Atom Pairs
4839	**F10[P-Br]**	Frequency of P - Br at topological distance 10	2D Atom Pairs
4840	**F10[P-I]**	Frequency of P - I at topological distance 10	2D Atom Pairs
4841	**F10[P-B]**	Frequency of P - B at topological distance 10	2D Atom Pairs
4842	**F10[P-Si]**	Frequency of P - Si at topological distance 10	2D Atom Pairs
4843	**F10[P-X]**	Frequency of P - X at topological distance 10	2D Atom Pairs
4844	**F10[F-F]**	Frequency of F - F at topological distance 10	2D Atom Pairs
4845	**F10[F-Cl]**	Frequency of F - Cl at topological distance 10	2D Atom Pairs
4846	**F10[F-Br]**	Frequency of F - Br at topological distance 10	2D Atom Pairs
4847	**F10[F-I]**	Frequency of F - I at topological distance 10	2D Atom Pairs
4848	**F10[F-B]**	Frequency of F - B at topological distance 10	2D Atom Pairs
4849	**F10[F-Si]**	Frequency of F - Si at topological distance 10	2D Atom Pairs
4850	**F10[F-X]**	Frequency of F - X at topological distance 10	2D Atom Pairs
4851	**F10[Cl-Cl]**	Frequency of Cl - Cl at topological distance 10	2D Atom Pairs
4852	**F10[Cl-Br]**	Frequency of Cl - Br at topological distance 10	2D Atom Pairs
4853	**F10[Cl-I]**	Frequency of Cl - I at topological distance 10	2D Atom Pairs
4854	**F10[Cl-B]**	Frequency of Cl - B at topological distance 10	2D Atom Pairs

No.	Name	Description	Block
4855	**F10[Cl-Si]**	Frequency of Cl - Si at topological distance 10	2D Atom Pairs
4856	**F10[Cl-X]**	Frequency of Cl - X at topological distance 10	2D Atom Pairs
4857	**F10[Br-Br]**	Frequency of Br - Br at topological distance 10	2D Atom Pairs
4858	**F10[Br-I]**	Frequency of Br - I at topological distance 10	2D Atom Pairs
4859	**F10[Br-B]**	Frequency of Br - B at topological distance 10	2D Atom Pairs
4860	**F10[Br-Si]**	Frequency of Br - Si at topological distance 10	2D Atom Pairs
4861	**F10[Br-X]**	Frequency of Br - X at topological distance 10	2D Atom Pairs
4862	**F10[I-I]**	Frequency of I - I at topological distance 10	2D Atom Pairs
4863	**F10[I-B]**	Frequency of I - B at topological distance 10	2D Atom Pairs
4864	**F10[I-Si]**	Frequency of I - Si at topological distance 10	2D Atom Pairs
4865	**F10[I-X]**	Frequency of I - X at topological distance 10	2D Atom Pairs
4866	**F10[B-B]**	Frequency of B - B at topological distance 10	2D Atom Pairs
4867	**F10[B-Si]**	Frequency of B - Si at topological distance 10	2D Atom Pairs
4868	**F10[B-X]**	Frequency of B - X at topological distance 10	2D Atom Pairs
4869	**F10[Si-Si]**	Frequency of Si - Si at topological distance 10	2D Atom Pairs
4870	**F10[Si-X]**	Frequency of Si - X at topological distance 10	2D Atom Pairs
4871	**F10[X-X]**	Frequency of X - X at topological distance 10	2D Atom Pairs
4872	**G(N..N)**	sum of geometrical distances between N..N	3D Atom Pairs
4873	**G(N..O)**	sum of geometrical distances between N..O	3D Atom Pairs
4874	**G(N..S)**	sum of geometrical distances between N..S	3D Atom Pairs
4875	**G(N..P)**	sum of geometrical distances between N..P	3D Atom Pairs
4876	**G(N..F)**	sum of geometrical distances between N..F	3D Atom Pairs
4877	**G(N..Cl)**	sum of geometrical distances between N..Cl	3D Atom Pairs
4878	**G(N..Br)**	sum of geometrical distances between N..Br	3D Atom Pairs
4879	**G(N..I)**	sum of geometrical distances between N..I	3D Atom Pairs
4880	**G(O..O)**	sum of geometrical distances between O..O	3D Atom Pairs
4881	**G(O..S)**	sum of geometrical distances between O..S	3D Atom Pairs
4882	**G(O..P)**	sum of geometrical distances between O..P	3D Atom Pairs
4883	**G(O..F)**	sum of geometrical distances between O..F	3D Atom Pairs
4884	**G(O..Cl)**	sum of geometrical distances between O..Cl	3D Atom Pairs
4885	**G(O..Br)**	sum of geometrical distances between O..Br	3D Atom Pairs
4886	**G(O..I)**	sum of geometrical distances between O..I	3D Atom Pairs

No.	Name	Description	Block
4887	**G(S..S)**	sum of geometrical distances between S..S	3D Atom Pairs
4888	**G(S..P)**	sum of geometrical distances between S..P	3D Atom Pairs
4889	**G(S..F)**	sum of geometrical distances between S..F	3D Atom Pairs
4890	**G(S..Cl)**	sum of geometrical distances between S..Cl	3D Atom Pairs
4891	**G(S..Br)**	sum of geometrical distances between S..Br	3D Atom Pairs
4892	**G(S..I)**	sum of geometrical distances between S..I	3D Atom Pairs
4893	**G(P..P)**	sum of geometrical distances between P..P	3D Atom Pairs
4894	**G(P..F)**	sum of geometrical distances between P..F	3D Atom Pairs
4895	**G(P..Cl)**	sum of geometrical distances between P..Cl	3D Atom Pairs
4896	**G(P..Br)**	sum of geometrical distances between P..Br	3D Atom Pairs
4897	**G(P..I)**	sum of geometrical distances between P..I	3D Atom Pairs
4898	**G(F..F)**	sum of geometrical distances between F..F	3D Atom Pairs
4899	**G(F..Cl)**	sum of geometrical distances between F..Cl	3D Atom Pairs
4900	**G(F..Br)**	sum of geometrical distances between F..Br	3D Atom Pairs
4901	**G(F..I)**	sum of geometrical distances between F..I	3D Atom Pairs
4902	**G(Cl..Cl)**	sum of geometrical distances between Cl..Cl	3D Atom Pairs
4903	**G(Cl..Br)**	sum of geometrical distances between Cl..Br	3D Atom Pairs
4904	**G(Cl..I)**	sum of geometrical distances between Cl..I	3D Atom Pairs
4905	**G(Br..Br)**	sum of geometrical distances between Br..Br	3D Atom Pairs
4906	**G(Br..I)**	sum of geometrical distances between Br..I	3D Atom Pairs
4907	**G(I..I)**	sum of geometrical distances between I..I	3D Atom Pairs
4908	**qpmax**	maximum positive charge	Charge descriptors
4909	**qnmax**	maximum negative charge	Charge descriptors
4910	**Qpos**	total positive charge	Charge descriptors
4911	**Qneg**	total negative charge	Charge descriptors
4912	**Qtot**	total absolute charge (electronic charge index - ECI)	Charge descriptors
4913	**Qmean**	mean absolute charge (charge polarization)	Charge descriptors
4914	**Q2**	total squared charge	Charge descriptors

No.	Name	Description	Block
4915	**RPCG**	relative positive charge	Charge descriptors
4916	**RNCG**	relative negative charge	Charge descriptors
4917	**SPP**	submolecular polarity parameter	Charge descriptors
4918	**TE1**	topographic electronic descriptor	Charge descriptors
4919	**TE2**	topographic electronic descriptor (bond resctricted)	Charge descriptors
4920	**PCWTE1**	partial charge weighted topological electronic index	Charge descriptors
4921	**PCWTE2**	partial charge weighted topological electronic index (bond resctricted)	Charge descriptors
4922	**LDI**	local dipole index	Charge descriptors
4923	**Uc**	unsaturation count	Molecular properties
4924	**Ui**	unsaturation index	Molecular properties
4925	**Hy**	hydrophilic factor	Molecular properties
4926	**AMR**	Ghose-Crippen molar refractivity	Molecular properties
4927	**TPSA(NO)**	topological polar surface area using N,O polar contributions	Molecular properties
4928	**TPSA(Tot)**	topological polar surface area using N,O,S,P polar contributions	Molecular properties
4929	**MLOGP**	Moriguchi octanol-water partition coeff. (logP)	Molecular properties
4930	**MLOGP2**	squared Moriguchi octanol-water partition coeff. (logP^2)	Molecular properties
4931	**ALOGP**	Ghose-Crippen octanol-water partition coeff. (logP)	Molecular properties
4932	**ALOGP2**	squared Ghose-Crippen octanol-water partition coeff. (logP^2)	Molecular properties
4933	**SAtot**	total surface area from P_VSA-like descriptors	Molecular properties

No.	Name	Description	Block
4934	**SAacc**	surface area of acceptor atoms from P_VSA-like descriptors	Molecular properties
4935	**SAdon**	surface area of donor atoms from P_VSA-like descriptors	Molecular properties
4936	**Vx**	McGowan volume	Molecular properties
4937	**VvdwMG**	van der Waals volume from McGowan volume	Molecular properties
4938	**VvdwZAZ**	van der Waals volume from Zhao-Abraham-Zissimos equation	Molecular properties
4939	**PDI**	packing density index	Molecular properties
4940	**BLTF96**	Verhaar Fish base-line toxicity from MLOGP (mmol/l)	Molecular properties
4941	**BLTD48**	Verhaar Daphnia base-line toxicity from MLOGP (mmol/l)	Molecular properties
4942	**BLTA96**	Verhaar Algae base-line toxicity from MLOGP (mmol/l)	Molecular properties
4943	**Ro5**	Lipinski Rule of 5	Drug-like indices
4944	**cRo5**	Complementary Lipinski Alert index	Drug-like indices
4945	**DLS_01**	modified drug-like score from Lipinski (4 rules)	Drug-like indices
4946	**DLS_02**	modified drug-like score from Oprea et al. (6 rules)	Drug-like indices
4947	**DLS_03**	modified drug-like score from Walters et al. (6 rules)	Drug-like indices
4948	**DLS_04**	modified drug-like score from Chen et al. (7 rules)	Drug-like indices
4949	**DLS_05**	modified drug-like score from Zheng et al. (2 rules)	Drug-like indices
4950	**DLS_06**	modified drug-like score from Rishton (6 rules)	Drug-like indices
4951	**DLS_07**	modified drug-like score from Veber et al. (2 rules)	Drug-like indices
4952	**DLS_cons**	DRAGON consensus drug-like score	Drug-like indices

No.	Name	Description	Block
4953	**LLS_01**	modified lead-like score from Congreve et al. (6 rules)	Drug-like indices
4954	**LLS_02**	modified lead-like score from Monge et al. (8 rules)	Drug-like indices
4955	**CMC-80**	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 80%	Drug-like indices
4956	**CMC-50**	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 50%	Drug-like indices
4957	**Inflammat-80**	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80%	Drug-like indices
4958	**Inflammat-50**	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50%	Drug-like indices
4959	**Depressant-80**	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80%	Drug-like indices
4960	**Depressant-50**	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50%	Drug-like indices
4961	**Psychotic-80**	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80%	Drug-like indices
4962	**Psychotic-50**	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50%	Drug-like indices
4963	**Hypertens-80**	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80%	Drug-like indices
4964	**Hypertens-50**	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50%	Drug-like indices
4965	**Hypnotic-80**	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80%	Drug-like indices
4966	**Hypnotic-50**	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50%	Drug-like indices
4967	**Neoplastic-80**	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80%	Drug-like indices
4968	**Neoplastic-50**	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50%	Drug-like indices
4969	**Infective-80**	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80%	Drug-like indices
4970	**Infective-50**	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50%	Drug-like indices
4971	**CATS3D_00_DD**	CATS3D Donor-Donor BIN 00 (0.000 - 1.000 Å)	CATS 3D
4972	**CATS3D_01_DD**	CATS3D Donor-Donor BIN 01 (1.000 - 2.000 Å)	CATS 3D
4973	**CATS3D_02_DD**	CATS3D Donor-Donor BIN 02 (2.000 - 3.000 Å)	CATS 3D

No.	Name	Description	Block
4974	**CATS3D_03_DD**	CATS3D Donor-Donor BIN 03 (3.000 - 4.000 Å)	CATS 3D
4975	**CATS3D_04_DD**	CATS3D Donor-Donor BIN 04 (4.000 - 5.000 Å)	CATS 3D
4976	**CATS3D_05_DD**	CATS3D Donor-Donor BIN 05 (5.000 - 6.000 Å)	CATS 3D
4977	**CATS3D_06_DD**	CATS3D Donor-Donor BIN 06 (6.000 - 7.000 Å)	CATS 3D
4978	**CATS3D_07_DD**	CATS3D Donor-Donor BIN 07 (7.000 - 8.000 Å)	CATS 3D
4979	**CATS3D_08_DD**	CATS3D Donor-Donor BIN 08 (8.000 - 9.000 Å)	CATS 3D
4980	**CATS3D_09_DD**	CATS3D Donor-Donor BIN 09 (9.000 - 10.000 Å)	CATS 3D
4981	**CATS3D_10_DD**	CATS3D Donor-Donor BIN 10 (10.000 - 11.000 Å)	CATS 3D
4982	**CATS3D_11_DD**	CATS3D Donor-Donor BIN 11 (11.000 - 12.000 Å)	CATS 3D
4983	**CATS3D_12_DD**	CATS3D Donor-Donor BIN 12 (12.000 - 13.000 Å)	CATS 3D
4984	**CATS3D_13_DD**	CATS3D Donor-Donor BIN 13 (13.000 - 14.000 Å)	CATS 3D
4985	**CATS3D_14_DD**	CATS3D Donor-Donor BIN 14 (14.000 - 15.000 Å)	CATS 3D
4986	**CATS3D_15_DD**	CATS3D Donor-Donor BIN 15 (15.000 - 16.000 Å)	CATS 3D
4987	**CATS3D_16_DD**	CATS3D Donor-Donor BIN 16 (16.000 - 17.000 Å)	CATS 3D
4988	**CATS3D_17_DD**	CATS3D Donor-Donor BIN 17 (17.000 - 18.000 Å)	CATS 3D
4989	**CATS3D_18_DD**	CATS3D Donor-Donor BIN 18 (18.000 - 19.000 Å)	CATS 3D
4990	**CATS3D_19_DD**	CATS3D Donor-Donor BIN 19 (19.000 - 20.000 Å)	CATS 3D
4991	**CATS3D_00_DA**	CATS3D Donor-Acceptor BIN 00 (0.000 - 1.000 Å)	CATS 3D
4992	**CATS3D_01_DA**	CATS3D Donor-Acceptor BIN 01 (1.000 - 2.000 Å)	CATS 3D
4993	**CATS3D_02_DA**	CATS3D Donor-Acceptor BIN 02 (2.000 - 3.000 Å)	CATS 3D
4994	**CATS3D_03_DA**	CATS3D Donor-Acceptor BIN 03 (3.000 - 4.000 Å)	CATS 3D
4995	**CATS3D_04_DA**	CATS3D Donor-Acceptor BIN 04 (4.000 - 5.000 Å)	CATS 3D
4996	**CATS3D_05_DA**	CATS3D Donor-Acceptor BIN 05 (5.000 - 6.000 Å)	CATS 3D
4997	**CATS3D_06_DA**	CATS3D Donor-Acceptor BIN 06 (6.000 - 7.000 Å)	CATS 3D
4998	**CATS3D_07_DA**	CATS3D Donor-Acceptor BIN 07 (7.000 - 8.000 Å)	CATS 3D
4999	**CATS3D_08_DA**	CATS3D Donor-Acceptor BIN 08 (8.000 - 9.000 Å)	CATS 3D
5000	**CATS3D_09_DA**	CATS3D Donor-Acceptor BIN 09 (9.000 - 10.000 Å)	CATS 3D
5001	**CATS3D_10_DA**	CATS3D Donor-Acceptor BIN 10 (10.000 - 11.000 Å)	CATS 3D
5002	**CATS3D_11_DA**	CATS3D Donor-Acceptor BIN 11 (11.000 - 12.000 Å)	CATS 3D
5003	**CATS3D_12_DA**	CATS3D Donor-Acceptor BIN 12 (12.000 - 13.000 Å)	CATS 3D
5004	**CATS3D_13_DA**	CATS3D Donor-Acceptor BIN 13 (13.000 - 14.000 Å)	CATS 3D
5005	**CATS3D_14_DA**	CATS3D Donor-Acceptor BIN 14 (14.000 - 15.000 Å)	CATS 3D

No.	Name	Description	Block
5006	**CATS3D_15_DA**	CATS3D Donor-Acceptor BIN 15 (15.000 - 16.000 Å)	CATS 3D
5007	**CATS3D_16_DA**	CATS3D Donor-Acceptor BIN 16 (16.000 - 17.000 Å)	CATS 3D
5008	**CATS3D_17_DA**	CATS3D Donor-Acceptor BIN 17 (17.000 - 18.000 Å)	CATS 3D
5009	**CATS3D_18_DA**	CATS3D Donor-Acceptor BIN 18 (18.000 - 19.000 Å)	CATS 3D
5010	**CATS3D_19_DA**	CATS3D Donor-Acceptor BIN 19 (19.000 - 20.000 Å)	CATS 3D
5011	**CATS3D_00_DP**	CATS3D Donor-Positive BIN 00 (0.000 - 1.000 Å)	CATS 3D
5012	**CATS3D_01_DP**	CATS3D Donor-Positive BIN 01 (1.000 - 2.000 Å)	CATS 3D
5013	**CATS3D_02_DP**	CATS3D Donor-Positive BIN 02 (2.000 - 3.000 Å)	CATS 3D
5014	**CATS3D_03_DP**	CATS3D Donor-Positive BIN 03 (3.000 - 4.000 Å)	CATS 3D
5015	**CATS3D_04_DP**	CATS3D Donor-Positive BIN 04 (4.000 - 5.000 Å)	CATS 3D
5016	**CATS3D_05_DP**	CATS3D Donor-Positive BIN 05 (5.000 - 6.000 Å)	CATS 3D
5017	**CATS3D_06_DP**	CATS3D Donor-Positive BIN 06 (6.000 - 7.000 Å)	CATS 3D
5018	**CATS3D_07_DP**	CATS3D Donor-Positive BIN 07 (7.000 - 8.000 Å)	CATS 3D
5019	**CATS3D_08_DP**	CATS3D Donor-Positive BIN 08 (8.000 - 9.000 Å)	CATS 3D
5020	**CATS3D_09_DP**	CATS3D Donor-Positive BIN 09 (9.000 - 10.000 Å)	CATS 3D
5021	**CATS3D_10_DP**	CATS3D Donor-Positive BIN 10 (10.000 - 11.000 Å)	CATS 3D
5022	**CATS3D_11_DP**	CATS3D Donor-Positive BIN 11 (11.000 - 12.000 Å)	CATS 3D
5023	**CATS3D_12_DP**	CATS3D Donor-Positive BIN 12 (12.000 - 13.000 Å)	CATS 3D
5024	**CATS3D_13_DP**	CATS3D Donor-Positive BIN 13 (13.000 - 14.000 Å)	CATS 3D
5025	**CATS3D_14_DP**	CATS3D Donor-Positive BIN 14 (14.000 - 15.000 Å)	CATS 3D
5026	**CATS3D_15_DP**	CATS3D Donor-Positive BIN 15 (15.000 - 16.000 Å)	CATS 3D
5027	**CATS3D_16_DP**	CATS3D Donor-Positive BIN 16 (16.000 - 17.000 Å)	CATS 3D
5028	**CATS3D_17_DP**	CATS3D Donor-Positive BIN 17 (17.000 - 18.000 Å)	CATS 3D
5029	**CATS3D_18_DP**	CATS3D Donor-Positive BIN 18 (18.000 - 19.000 Å)	CATS 3D
5030	**CATS3D_19_DP**	CATS3D Donor-Positive BIN 19 (19.000 - 20.000 Å)	CATS 3D
5031	**CATS3D_00_DN**	CATS3D Donor-Negative BIN 00 (0.000 - 1.000 Å)	CATS 3D
5032	**CATS3D_01_DN**	CATS3D Donor-Negative BIN 01 (1.000 - 2.000 Å)	CATS 3D
5033	**CATS3D_02_DN**	CATS3D Donor-Negative BIN 02 (2.000 - 3.000 Å)	CATS 3D
5034	**CATS3D_03_DN**	CATS3D Donor-Negative BIN 03 (3.000 - 4.000 Å)	CATS 3D
5035	**CATS3D_04_DN**	CATS3D Donor-Negative BIN 04 (4.000 - 5.000 Å)	CATS 3D
5036	**CATS3D_05_DN**	CATS3D Donor-Negative BIN 05 (5.000 - 6.000 Å)	CATS 3D
5037	**CATS3D_06_DN**	CATS3D Donor-Negative BIN 06 (6.000 - 7.000 Å)	CATS 3D

No.	Name	Description	Block
5038	**CATS3D_07_DN**	CATS3D Donor-Negative BIN 07 (7.000 - 8.000 Å)	CATS 3D
5039	**CATS3D_08_DN**	CATS3D Donor-Negative BIN 08 (8.000 - 9.000 Å)	CATS 3D
5040	**CATS3D_09_DN**	CATS3D Donor-Negative BIN 09 (9.000 - 10.000 Å)	CATS 3D
5041	**CATS3D_10_DN**	CATS3D Donor-Negative BIN 10 (10.000 - 11.000 Å)	CATS 3D
5042	**CATS3D_11_DN**	CATS3D Donor-Negative BIN 11 (11.000 - 12.000 Å)	CATS 3D
5043	**CATS3D_12_DN**	CATS3D Donor-Negative BIN 12 (12.000 - 13.000 Å)	CATS 3D
5044	**CATS3D_13_DN**	CATS3D Donor-Negative BIN 13 (13.000 - 14.000 Å)	CATS 3D
5045	**CATS3D_14_DN**	CATS3D Donor-Negative BIN 14 (14.000 - 15.000 Å)	CATS 3D
5046	**CATS3D_15_DN**	CATS3D Donor-Negative BIN 15 (15.000 - 16.000 Å)	CATS 3D
5047	**CATS3D_16_DN**	CATS3D Donor-Negative BIN 16 (16.000 - 17.000 Å)	CATS 3D
5048	**CATS3D_17_DN**	CATS3D Donor-Negative BIN 17 (17.000 - 18.000 Å)	CATS 3D
5049	**CATS3D_18_DN**	CATS3D Donor-Negative BIN 18 (18.000 - 19.000 Å)	CATS 3D
5050	**CATS3D_19_DN**	CATS3D Donor-Negative BIN 19 (19.000 - 20.000 Å)	CATS 3D
5051	**CATS3D_00_DL**	CATS3D Donor-Lipophilic BIN 00 (0.000 - 1.000 Å)	CATS 3D
5052	**CATS3D_01_DL**	CATS3D Donor-Lipophilic BIN 01 (1.000 - 2.000 Å)	CATS 3D
5053	**CATS3D_02_DL**	CATS3D Donor-Lipophilic BIN 02 (2.000 - 3.000 Å)	CATS 3D
5054	**CATS3D_03_DL**	CATS3D Donor-Lipophilic BIN 03 (3.000 - 4.000 Å)	CATS 3D
5055	**CATS3D_04_DL**	CATS3D Donor-Lipophilic BIN 04 (4.000 - 5.000 Å)	CATS 3D
5056	**CATS3D_05_DL**	CATS3D Donor-Lipophilic BIN 05 (5.000 - 6.000 Å)	CATS 3D
5057	**CATS3D_06_DL**	CATS3D Donor-Lipophilic BIN 06 (6.000 - 7.000 Å)	CATS 3D
5058	**CATS3D_07_DL**	CATS3D Donor-Lipophilic BIN 07 (7.000 - 8.000 Å)	CATS 3D
5059	**CATS3D_08_DL**	CATS3D Donor-Lipophilic BIN 08 (8.000 - 9.000 Å)	CATS 3D
5060	**CATS3D_09_DL**	CATS3D Donor-Lipophilic BIN 09 (9.000 - 10.000 Å)	CATS 3D
5061	**CATS3D_10_DL**	CATS3D Donor-Lipophilic BIN 10 (10.000 - 11.000 Å)	CATS 3D
5062	**CATS3D_11_DL**	CATS3D Donor-Lipophilic BIN 11 (11.000 - 12.000 Å)	CATS 3D
5063	**CATS3D_12_DL**	CATS3D Donor-Lipophilic BIN 12 (12.000 - 13.000 Å)	CATS 3D
5064	**CATS3D_13_DL**	CATS3D Donor-Lipophilic BIN 13 (13.000 - 14.000 Å)	CATS 3D
5065	**CATS3D_14_DL**	CATS3D Donor-Lipophilic BIN 14 (14.000 - 15.000 Å)	CATS 3D
5066	**CATS3D_15_DL**	CATS3D Donor-Lipophilic BIN 15 (15.000 - 16.000 Å)	CATS 3D
5067	**CATS3D_16_DL**	CATS3D Donor-Lipophilic BIN 16 (16.000 - 17.000 Å)	CATS 3D
5068	**CATS3D_17_DL**	CATS3D Donor-Lipophilic BIN 17 (17.000 - 18.000 Å)	CATS 3D
5069	**CATS3D_18_DL**	CATS3D Donor-Lipophilic BIN 18 (18.000 - 19.000 Å)	CATS 3D

No.	Name	Description	Block
5070	**CATS3D_19_DL**	CATS3D Donor-Lipophilic BIN 19 (19.000 - 20.000 Å)	CATS 3D
5071	**CATS3D_00_AA**	CATS3D Acceptor-Acceptor BIN 00 (0.000 - 1.000 Å)	CATS 3D
5072	**CATS3D_01_AA**	CATS3D Acceptor-Acceptor BIN 01 (1.000 - 2.000 Å)	CATS 3D
5073	**CATS3D_02_AA**	CATS3D Acceptor-Acceptor BIN 02 (2.000 - 3.000 Å)	CATS 3D
5074	**CATS3D_03_AA**	CATS3D Acceptor-Acceptor BIN 03 (3.000 - 4.000 Å)	CATS 3D
5075	**CATS3D_04_AA**	CATS3D Acceptor-Acceptor BIN 04 (4.000 - 5.000 Å)	CATS 3D
5076	**CATS3D_05_AA**	CATS3D Acceptor-Acceptor BIN 05 (5.000 - 6.000 Å)	CATS 3D
5077	**CATS3D_06_AA**	CATS3D Acceptor-Acceptor BIN 06 (6.000 - 7.000 Å)	CATS 3D
5078	**CATS3D_07_AA**	CATS3D Acceptor-Acceptor BIN 07 (7.000 - 8.000 Å)	CATS 3D
5079	**CATS3D_08_AA**	CATS3D Acceptor-Acceptor BIN 08 (8.000 - 9.000 Å)	CATS 3D
5080	**CATS3D_09_AA**	CATS3D Acceptor-Acceptor BIN 09 (9.000 - 10.000 Å)	CATS 3D
5081	**CATS3D_10_AA**	CATS3D Acceptor-Acceptor BIN 10 (10.000 - 11.000 Å)	CATS 3D
5082	**CATS3D_11_AA**	CATS3D Acceptor-Acceptor BIN 11 (11.000 - 12.000 Å)	CATS 3D
5083	**CATS3D_12_AA**	CATS3D Acceptor-Acceptor BIN 12 (12.000 - 13.000 Å)	CATS 3D
5084	**CATS3D_13_AA**	CATS3D Acceptor-Acceptor BIN 13 (13.000 - 14.000 Å)	CATS 3D
5085	**CATS3D_14_AA**	CATS3D Acceptor-Acceptor BIN 14 (14.000 - 15.000 Å)	CATS 3D
5086	**CATS3D_15_AA**	CATS3D Acceptor-Acceptor BIN 15 (15.000 - 16.000 Å)	CATS 3D
5087	**CATS3D_16_AA**	CATS3D Acceptor-Acceptor BIN 16 (16.000 - 17.000 Å)	CATS 3D
5088	**CATS3D_17_AA**	CATS3D Acceptor-Acceptor BIN 17 (17.000 - 18.000 Å)	CATS 3D
5089	**CATS3D_18_AA**	CATS3D Acceptor-Acceptor BIN 18 (18.000 - 19.000 Å)	CATS 3D
5090	**CATS3D_19_AA**	CATS3D Acceptor-Acceptor BIN 19 (19.000 - 20.000 Å)	CATS 3D
5091	**CATS3D_00_AP**	CATS3D Acceptor-Positive BIN 00 (0.000 - 1.000 Å)	CATS 3D
5092	**CATS3D_01_AP**	CATS3D Acceptor-Positive BIN 01 (1.000 - 2.000 Å)	CATS 3D
5093	**CATS3D_02_AP**	CATS3D Acceptor-Positive BIN 02 (2.000 - 3.000 Å)	CATS 3D
5094	**CATS3D_03_AP**	CATS3D Acceptor-Positive BIN 03 (3.000 - 4.000 Å)	CATS 3D
5095	**CATS3D_04_AP**	CATS3D Acceptor-Positive BIN 04 (4.000 - 5.000 Å)	CATS 3D
5096	**CATS3D_05_AP**	CATS3D Acceptor-Positive BIN 05 (5.000 - 6.000 Å)	CATS 3D
5097	**CATS3D_06_AP**	CATS3D Acceptor-Positive BIN 06 (6.000 - 7.000 Å)	CATS 3D
5098	**CATS3D_07_AP**	CATS3D Acceptor-Positive BIN 07 (7.000 - 8.000 Å)	CATS 3D
5099	**CATS3D_08_AP**	CATS3D Acceptor-Positive BIN 08 (8.000 - 9.000 Å)	CATS 3D
5100	**CATS3D_09_AP**	CATS3D Acceptor-Positive BIN 09 (9.000 - 10.000 Å)	CATS 3D
5101	**CATS3D_10_AP**	CATS3D Acceptor-Positive BIN 10 (10.000 - 11.000 Å)	CATS 3D

No.	Name	Description	Block
5102	**CATS3D_11_AP**	CATS3D Acceptor-Positive BIN 11 (11.000 - 12.000 Å)	CATS 3D
5103	**CATS3D_12_AP**	CATS3D Acceptor-Positive BIN 12 (12.000 - 13.000 Å)	CATS 3D
5104	**CATS3D_13_AP**	CATS3D Acceptor-Positive BIN 13 (13.000 - 14.000 Å)	CATS 3D
5105	**CATS3D_14_AP**	CATS3D Acceptor-Positive BIN 14 (14.000 - 15.000 Å)	CATS 3D
5106	**CATS3D_15_AP**	CATS3D Acceptor-Positive BIN 15 (15.000 - 16.000 Å)	CATS 3D
5107	**CATS3D_16_AP**	CATS3D Acceptor-Positive BIN 16 (16.000 - 17.000 Å)	CATS 3D
5108	**CATS3D_17_AP**	CATS3D Acceptor-Positive BIN 17 (17.000 - 18.000 Å)	CATS 3D
5109	**CATS3D_18_AP**	CATS3D Acceptor-Positive BIN 18 (18.000 - 19.000 Å)	CATS 3D
5110	**CATS3D_19_AP**	CATS3D Acceptor-Positive BIN 19 (19.000 - 20.000 Å)	CATS 3D
5111	**CATS3D_00_AN**	CATS3D Acceptor-Negative BIN 00 (0.000 - 1.000 Å)	CATS 3D
5112	**CATS3D_01_AN**	CATS3D Acceptor-Negative BIN 01 (1.000 - 2.000 Å)	CATS 3D
5113	**CATS3D_02_AN**	CATS3D Acceptor-Negative BIN 02 (2.000 - 3.000 Å)	CATS 3D
5114	**CATS3D_03_AN**	CATS3D Acceptor-Negative BIN 03 (3.000 - 4.000 Å)	CATS 3D
5115	**CATS3D_04_AN**	CATS3D Acceptor-Negative BIN 04 (4.000 - 5.000 Å)	CATS 3D
5116	**CATS3D_05_AN**	CATS3D Acceptor-Negative BIN 05 (5.000 - 6.000 Å)	CATS 3D
5117	**CATS3D_06_AN**	CATS3D Acceptor-Negative BIN 06 (6.000 - 7.000 Å)	CATS 3D
5118	**CATS3D_07_AN**	CATS3D Acceptor-Negative BIN 07 (7.000 - 8.000 Å)	CATS 3D
5119	**CATS3D_08_AN**	CATS3D Acceptor-Negative BIN 08 (8.000 - 9.000 Å)	CATS 3D
5120	**CATS3D_09_AN**	CATS3D Acceptor-Negative BIN 09 (9.000 - 10.000 Å)	CATS 3D
5121	**CATS3D_10_AN**	CATS3D Acceptor-Negative BIN 10 (10.000 - 11.000 Å)	CATS 3D
5122	**CATS3D_11_AN**	CATS3D Acceptor-Negative BIN 11 (11.000 - 12.000 Å)	CATS 3D
5123	**CATS3D_12_AN**	CATS3D Acceptor-Negative BIN 12 (12.000 - 13.000 Å)	CATS 3D
5124	**CATS3D_13_AN**	CATS3D Acceptor-Negative BIN 13 (13.000 - 14.000 Å)	CATS 3D
5125	**CATS3D_14_AN**	CATS3D Acceptor-Negative BIN 14 (14.000 - 15.000 Å)	CATS 3D
5126	**CATS3D_15_AN**	CATS3D Acceptor-Negative BIN 15 (15.000 - 16.000 Å)	CATS 3D
5127	**CATS3D_16_AN**	CATS3D Acceptor-Negative BIN 16 (16.000 - 17.000 Å)	CATS 3D
5128	**CATS3D_17_AN**	CATS3D Acceptor-Negative BIN 17 (17.000 - 18.000 Å)	CATS 3D
5129	**CATS3D_18_AN**	CATS3D Acceptor-Negative BIN 18 (18.000 - 19.000 Å)	CATS 3D
5130	**CATS3D_19_AN**	CATS3D Acceptor-Negative BIN 19 (19.000 - 20.000 Å)	CATS 3D
5131	**CATS3D_00_AL**	CATS3D Acceptor-Lipophilic BIN 00 (0.000 - 1.000 Å)	CATS 3D
5132	**CATS3D_01_AL**	CATS3D Acceptor-Lipophilic BIN 01 (1.000 - 2.000 Å)	CATS 3D
5133	**CATS3D_02_AL**	CATS3D Acceptor-Lipophilic BIN 02 (2.000 - 3.000 Å)	CATS 3D

No.	Name	Description	Block
5134	**CATS3D_03_AL**	CATS3D Acceptor-Lipophilic BIN 03 (3.000 - 4.000 Å)	CATS 3D
5135	**CATS3D_04_AL**	CATS3D Acceptor-Lipophilic BIN 04 (4.000 - 5.000 Å)	CATS 3D
5136	**CATS3D_05_AL**	CATS3D Acceptor-Lipophilic BIN 05 (5.000 - 6.000 Å)	CATS 3D
5137	**CATS3D_06_AL**	CATS3D Acceptor-Lipophilic BIN 06 (6.000 - 7.000 Å)	CATS 3D
5138	**CATS3D_07_AL**	CATS3D Acceptor-Lipophilic BIN 07 (7.000 - 8.000 Å)	CATS 3D
5139	**CATS3D_08_AL**	CATS3D Acceptor-Lipophilic BIN 08 (8.000 - 9.000 Å)	CATS 3D
5140	**CATS3D_09_AL**	CATS3D Acceptor-Lipophilic BIN 09 (9.000 - 10.000 Å)	CATS 3D
5141	**CATS3D_10_AL**	CATS3D Acceptor-Lipophilic BIN 10 (10.000 - 11.000 Å)	CATS 3D
5142	**CATS3D_11_AL**	CATS3D Acceptor-Lipophilic BIN 11 (11.000 - 12.000 Å)	CATS 3D
5143	**CATS3D_12_AL**	CATS3D Acceptor-Lipophilic BIN 12 (12.000 - 13.000 Å)	CATS 3D
5144	**CATS3D_13_AL**	CATS3D Acceptor-Lipophilic BIN 13 (13.000 - 14.000 Å)	CATS 3D
5145	**CATS3D_14_AL**	CATS3D Acceptor-Lipophilic BIN 14 (14.000 - 15.000 Å)	CATS 3D
5146	**CATS3D_15_AL**	CATS3D Acceptor-Lipophilic BIN 15 (15.000 - 16.000 Å)	CATS 3D
5147	**CATS3D_16_AL**	CATS3D Acceptor-Lipophilic BIN 16 (16.000 - 17.000 Å)	CATS 3D
5148	**CATS3D_17_AL**	CATS3D Acceptor-Lipophilic BIN 17 (17.000 - 18.000 Å)	CATS 3D
5149	**CATS3D_18_AL**	CATS3D Acceptor-Lipophilic BIN 18 (18.000 - 19.000 Å)	CATS 3D
5150	**CATS3D_19_AL**	CATS3D Acceptor-Lipophilic BIN 19 (19.000 - 20.000 Å)	CATS 3D
5151	**CATS3D_00_PP**	CATS3D Positive-Positive BIN 00 (0.000 - 1.000 Å)	CATS 3D
5152	**CATS3D_01_PP**	CATS3D Positive-Positive BIN 01 (1.000 - 2.000 Å)	CATS 3D
5153	**CATS3D_02_PP**	CATS3D Positive-Positive BIN 02 (2.000 - 3.000 Å)	CATS 3D
5154	**CATS3D_03_PP**	CATS3D Positive-Positive BIN 03 (3.000 - 4.000 Å)	CATS 3D
5155	**CATS3D_04_PP**	CATS3D Positive-Positive BIN 04 (4.000 - 5.000 Å)	CATS 3D
5156	**CATS3D_05_PP**	CATS3D Positive-Positive BIN 05 (5.000 - 6.000 Å)	CATS 3D
5157	**CATS3D_06_PP**	CATS3D Positive-Positive BIN 06 (6.000 - 7.000 Å)	CATS 3D
5158	**CATS3D_07_PP**	CATS3D Positive-Positive BIN 07 (7.000 - 8.000 Å)	CATS 3D
5159	**CATS3D_08_PP**	CATS3D Positive-Positive BIN 08 (8.000 - 9.000 Å)	CATS 3D
5160	**CATS3D_09_PP**	CATS3D Positive-Positive BIN 09 (9.000 - 10.000 Å)	CATS 3D
5161	**CATS3D_10_PP**	CATS3D Positive-Positive BIN 10 (10.000 - 11.000 Å)	CATS 3D
5162	**CATS3D_11_PP**	CATS3D Positive-Positive BIN 11 (11.000 - 12.000 Å)	CATS 3D
5163	**CATS3D_12_PP**	CATS3D Positive-Positive BIN 12 (12.000 - 13.000 Å)	CATS 3D
5164	**CATS3D_13_PP**	CATS3D Positive-Positive BIN 13 (13.000 - 14.000 Å)	CATS 3D
5165	**CATS3D_14_PP**	CATS3D Positive-Positive BIN 14 (14.000 - 15.000 Å)	CATS 3D

No.	Name	Description	Block
5166	**CATS3D_15_PP**	CATS3D Positive-Positive BIN 15 (15.000 - 16.000 Å)	CATS 3D
5167	**CATS3D_16_PP**	CATS3D Positive-Positive BIN 16 (16.000 - 17.000 Å)	CATS 3D
5168	**CATS3D_17_PP**	CATS3D Positive-Positive BIN 17 (17.000 - 18.000 Å)	CATS 3D
5169	**CATS3D_18_PP**	CATS3D Positive-Positive BIN 18 (18.000 - 19.000 Å)	CATS 3D
5170	**CATS3D_19_PP**	CATS3D Positive-Positive BIN 19 (19.000 - 20.000 Å)	CATS 3D
5171	**CATS3D_00_PN**	CATS3D Positive-Negative BIN 00 (0.000 - 1.000 Å)	CATS 3D
5172	**CATS3D_01_PN**	CATS3D Positive-Negative BIN 01 (1.000 - 2.000 Å)	CATS 3D
5173	**CATS3D_02_PN**	CATS3D Positive-Negative BIN 02 (2.000 - 3.000 Å)	CATS 3D
5174	**CATS3D_03_PN**	CATS3D Positive-Negative BIN 03 (3.000 - 4.000 Å)	CATS 3D
5175	**CATS3D_04_PN**	CATS3D Positive-Negative BIN 04 (4.000 - 5.000 Å)	CATS 3D
5176	**CATS3D_05_PN**	CATS3D Positive-Negative BIN 05 (5.000 - 6.000 Å)	CATS 3D
5177	**CATS3D_06_PN**	CATS3D Positive-Negative BIN 06 (6.000 - 7.000 Å)	CATS 3D
5178	**CATS3D_07_PN**	CATS3D Positive-Negative BIN 07 (7.000 - 8.000 Å)	CATS 3D
5179	**CATS3D_08_PN**	CATS3D Positive-Negative BIN 08 (8.000 - 9.000 Å)	CATS 3D
5180	**CATS3D_09_PN**	CATS3D Positive-Negative BIN 09 (9.000 - 10.000 Å)	CATS 3D
5181	**CATS3D_10_PN**	CATS3D Positive-Negative BIN 10 (10.000 - 11.000 Å)	CATS 3D
5182	**CATS3D_11_PN**	CATS3D Positive-Negative BIN 11 (11.000 - 12.000 Å)	CATS 3D
5183	**CATS3D_12_PN**	CATS3D Positive-Negative BIN 12 (12.000 - 13.000 Å)	CATS 3D
5184	**CATS3D_13_PN**	CATS3D Positive-Negative BIN 13 (13.000 - 14.000 Å)	CATS 3D
5185	**CATS3D_14_PN**	CATS3D Positive-Negative BIN 14 (14.000 - 15.000 Å)	CATS 3D
5186	**CATS3D_15_PN**	CATS3D Positive-Negative BIN 15 (15.000 - 16.000 Å)	CATS 3D
5187	**CATS3D_16_PN**	CATS3D Positive-Negative BIN 16 (16.000 - 17.000 Å)	CATS 3D
5188	**CATS3D_17_PN**	CATS3D Positive-Negative BIN 17 (17.000 - 18.000 Å)	CATS 3D
5189	**CATS3D_18_PN**	CATS3D Positive-Negative BIN 18 (18.000 - 19.000 Å)	CATS 3D
5190	**CATS3D_19_PN**	CATS3D Positive-Negative BIN 19 (19.000 - 20.000 Å)	CATS 3D
5191	**CATS3D_00_PL**	CATS3D Positive-Lipophilic BIN 00 (0.000 - 1.000 Å)	CATS 3D
5192	**CATS3D_01_PL**	CATS3D Positive-Lipophilic BIN 01 (1.000 - 2.000 Å)	CATS 3D
5193	**CATS3D_02_PL**	CATS3D Positive-Lipophilic BIN 02 (2.000 - 3.000 Å)	CATS 3D
5194	**CATS3D_03_PL**	CATS3D Positive-Lipophilic BIN 03 (3.000 - 4.000 Å)	CATS 3D
5195	**CATS3D_04_PL**	CATS3D Positive-Lipophilic BIN 04 (4.000 - 5.000 Å)	CATS 3D
5196	**CATS3D_05_PL**	CATS3D Positive-Lipophilic BIN 05 (5.000 - 6.000 Å)	CATS 3D
5197	**CATS3D_06_PL**	CATS3D Positive-Lipophilic BIN 06 (6.000 - 7.000 Å)	CATS 3D

No.	Name	Description	Block
5198	**CATS3D_07_PL**	CATS3D Positive-Lipophilic BIN 07 (7.000 - 8.000 Å)	CATS 3D
5199	**CATS3D_08_PL**	CATS3D Positive-Lipophilic BIN 08 (8.000 - 9.000 Å)	CATS 3D
5200	**CATS3D_09_PL**	CATS3D Positive-Lipophilic BIN 09 (9.000 - 10.000 Å)	CATS 3D
5201	**CATS3D_10_PL**	CATS3D Positive-Lipophilic BIN 10 (10.000 - 11.000 Å)	CATS 3D
5202	**CATS3D_11_PL**	CATS3D Positive-Lipophilic BIN 11 (11.000 - 12.000 Å)	CATS 3D
5203	**CATS3D_12_PL**	CATS3D Positive-Lipophilic BIN 12 (12.000 - 13.000 Å)	CATS 3D
5204	**CATS3D_13_PL**	CATS3D Positive-Lipophilic BIN 13 (13.000 - 14.000 Å)	CATS 3D
5205	**CATS3D_14_PL**	CATS3D Positive-Lipophilic BIN 14 (14.000 - 15.000 Å)	CATS 3D
5206	**CATS3D_15_PL**	CATS3D Positive-Lipophilic BIN 15 (15.000 - 16.000 Å)	CATS 3D
5207	**CATS3D_16_PL**	CATS3D Positive-Lipophilic BIN 16 (16.000 - 17.000 Å)	CATS 3D
5208	**CATS3D_17_PL**	CATS3D Positive-Lipophilic BIN 17 (17.000 - 18.000 Å)	CATS 3D
5209	**CATS3D_18_PL**	CATS3D Positive-Lipophilic BIN 18 (18.000 - 19.000 Å)	CATS 3D
5210	**CATS3D_19_PL**	CATS3D Positive-Lipophilic BIN 19 (19.000 - 20.000 Å)	CATS 3D
5211	**CATS3D_00_NN**	CATS3D Negative-Negative BIN 00 (0.000 - 1.000 Å)	CATS 3D
5212	**CATS3D_01_NN**	CATS3D Negative-Negative BIN 01 (1.000 - 2.000 Å)	CATS 3D
5213	**CATS3D_02_NN**	CATS3D Negative-Negative BIN 02 (2.000 - 3.000 Å)	CATS 3D
5214	**CATS3D_03_NN**	CATS3D Negative-Negative BIN 03 (3.000 - 4.000 Å)	CATS 3D
5215	**CATS3D_04_NN**	CATS3D Negative-Negative BIN 04 (4.000 - 5.000 Å)	CATS 3D
5216	**CATS3D_05_NN**	CATS3D Negative-Negative BIN 05 (5.000 - 6.000 Å)	CATS 3D
5217	**CATS3D_06_NN**	CATS3D Negative-Negative BIN 06 (6.000 - 7.000 Å)	CATS 3D
5218	**CATS3D_07_NN**	CATS3D Negative-Negative BIN 07 (7.000 - 8.000 Å)	CATS 3D
5219	**CATS3D_08_NN**	CATS3D Negative-Negative BIN 08 (8.000 - 9.000 Å)	CATS 3D
5220	**CATS3D_09_NN**	CATS3D Negative-Negative BIN 09 (9.000 - 10.000 Å)	CATS 3D
5221	**CATS3D_10_NN**	CATS3D Negative-Negative BIN 10 (10.000 - 11.000 Å)	CATS 3D
5222	**CATS3D_11_NN**	CATS3D Negative-Negative BIN 11 (11.000 - 12.000 Å)	CATS 3D
5223	**CATS3D_12_NN**	CATS3D Negative-Negative BIN 12 (12.000 - 13.000 Å)	CATS 3D
5224	**CATS3D_13_NN**	CATS3D Negative-Negative BIN 13 (13.000 - 14.000 Å)	CATS 3D
5225	**CATS3D_14_NN**	CATS3D Negative-Negative BIN 14 (14.000 - 15.000 Å)	CATS 3D
5226	**CATS3D_15_NN**	CATS3D Negative-Negative BIN 15 (15.000 - 16.000 Å)	CATS 3D
5227	**CATS3D_16_NN**	CATS3D Negative-Negative BIN 16 (16.000 - 17.000 Å)	CATS 3D
5228	**CATS3D_17_NN**	CATS3D Negative-Negative BIN 17 (17.000 - 18.000 Å)	CATS 3D
5229	**CATS3D_18_NN**	CATS3D Negative-Negative BIN 18 (18.000 - 19.000 Å)	CATS 3D

No.	Name	Description	Block
5230	**CATS3D_19_NN**	CATS3D Negative-Negative BIN 19 (19.000 - 20.000 Å)	CATS 3D
5231	**CATS3D_00_NL**	CATS3D Negative-Lipophilic BIN 00 (0.000 - 1.000 Å)	CATS 3D
5232	**CATS3D_01_NL**	CATS3D Negative-Lipophilic BIN 01 (1.000 - 2.000 Å)	CATS 3D
5233	**CATS3D_02_NL**	CATS3D Negative-Lipophilic BIN 02 (2.000 - 3.000 Å)	CATS 3D
5234	**CATS3D_03_NL**	CATS3D Negative-Lipophilic BIN 03 (3.000 - 4.000 Å)	CATS 3D
5235	**CATS3D_04_NL**	CATS3D Negative-Lipophilic BIN 04 (4.000 - 5.000 Å)	CATS 3D
5236	**CATS3D_05_NL**	CATS3D Negative-Lipophilic BIN 05 (5.000 - 6.000 Å)	CATS 3D
5237	**CATS3D_06_NL**	CATS3D Negative-Lipophilic BIN 06 (6.000 - 7.000 Å)	CATS 3D
5238	**CATS3D_07_NL**	CATS3D Negative-Lipophilic BIN 07 (7.000 - 8.000 Å)	CATS 3D
5239	**CATS3D_08_NL**	CATS3D Negative-Lipophilic BIN 08 (8.000 - 9.000 Å)	CATS 3D
5240	**CATS3D_09_NL**	CATS3D Negative-Lipophilic BIN 09 (9.000 - 10.000 Å)	CATS 3D
5241	**CATS3D_10_NL**	CATS3D Negative-Lipophilic BIN 10 (10.000 - 11.000 Å)	CATS 3D
5242	**CATS3D_11_NL**	CATS3D Negative-Lipophilic BIN 11 (11.000 - 12.000 Å)	CATS 3D
5243	**CATS3D_12_NL**	CATS3D Negative-Lipophilic BIN 12 (12.000 - 13.000 Å)	CATS 3D
5244	**CATS3D_13_NL**	CATS3D Negative-Lipophilic BIN 13 (13.000 - 14.000 Å)	CATS 3D
5245	**CATS3D_14_NL**	CATS3D Negative-Lipophilic BIN 14 (14.000 - 15.000 Å)	CATS 3D
5246	**CATS3D_15_NL**	CATS3D Negative-Lipophilic BIN 15 (15.000 - 16.000 Å)	CATS 3D
5247	**CATS3D_16_NL**	CATS3D Negative-Lipophilic BIN 16 (16.000 - 17.000 Å)	CATS 3D
5248	**CATS3D_17_NL**	CATS3D Negative-Lipophilic BIN 17 (17.000 - 18.000 Å)	CATS 3D
5249	**CATS3D_18_NL**	CATS3D Negative-Lipophilic BIN 18 (18.000 - 19.000 Å)	CATS 3D
5250	**CATS3D_19_NL**	CATS3D Negative-Lipophilic BIN 19 (19.000 - 20.000 Å)	CATS 3D
5251	**CATS3D_00_LL**	CATS3D Lipophilic-Lipophilic BIN 00 (0.000 - 1.000 Å)	CATS 3D
5252	**CATS3D_01_LL**	CATS3D Lipophilic-Lipophilic BIN 01 (1.000 - 2.000 Å)	CATS 3D
5253	**CATS3D_02_LL**	CATS3D Lipophilic-Lipophilic BIN 02 (2.000 - 3.000 Å)	CATS 3D
5254	**CATS3D_03_LL**	CATS3D Lipophilic-Lipophilic BIN 03 (3.000 - 4.000 Å)	CATS 3D
5255	**CATS3D_04_LL**	CATS3D Lipophilic-Lipophilic BIN 04 (4.000 - 5.000 Å)	CATS 3D
5256	**CATS3D_05_LL**	CATS3D Lipophilic-Lipophilic BIN 05 (5.000 - 6.000 Å)	CATS 3D
5257	**CATS3D_06_LL**	CATS3D Lipophilic-Lipophilic BIN 06 (6.000 - 7.000 Å)	CATS 3D
5258	**CATS3D_07_LL**	CATS3D Lipophilic-Lipophilic BIN 07 (7.000 - 8.000 Å)	CATS 3D
5259	**CATS3D_08_LL**	CATS3D Lipophilic-Lipophilic BIN 08 (8.000 - 9.000 Å)	CATS 3D
5260	**CATS3D_09_LL**	CATS3D Lipophilic-Lipophilic BIN 09 (9.000 - 10.000 Å)	CATS 3D
5261	**CATS3D_10_LL**	CATS3D Lipophilic-Lipophilic BIN 10 (10.000 - 11.000 Å)	CATS 3D

No.	Name	Description	Block
5262	**CATS3D_11_LL**	CATS3D Lipophilic-Lipophilic BIN 11 (11.000 - 12.000 Å)	CATS 3D
5263	**CATS3D_12_LL**	CATS3D Lipophilic-Lipophilic BIN 12 (12.000 - 13.000 Å)	CATS 3D
5264	**CATS3D_13_LL**	CATS3D Lipophilic-Lipophilic BIN 13 (13.000 - 14.000 Å)	CATS 3D
5265	**CATS3D_14_LL**	CATS3D Lipophilic-Lipophilic BIN 14 (14.000 - 15.000 Å)	CATS 3D
5266	**CATS3D_15_LL**	CATS3D Lipophilic-Lipophilic BIN 15 (15.000 - 16.000 Å)	CATS 3D
5267	**CATS3D_16_LL**	CATS3D Lipophilic-Lipophilic BIN 16 (16.000 - 17.000 Å)	CATS 3D
5268	**CATS3D_17_LL**	CATS3D Lipophilic-Lipophilic BIN 17 (17.000 - 18.000 Å)	CATS 3D
5269	**CATS3D_18_LL**	CATS3D Lipophilic-Lipophilic BIN 18 (18.000 - 19.000 Å)	CATS 3D
5270	**CATS3D_19_LL**	CATS3D Lipophilic-Lipophilic BIN 19 (19.000 - 20.000 Å)	CATS 3D