1. Constitutional indices

No.	Name	Description
1	MW	molecular weight
2	AMW	average molecular weight
3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)
4	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)
5	Sp	sum of atomic polarizabilities (scaled on Carbon atom)
6	Si	sum of first ionization potentials (scaled on Carbon atom)
7	Mv	mean atomic van der Waals volume (scaled on Carbon atom)
8	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)
9	Mp	mean atomic polarizability (scaled on Carbon atom)
10	Mi	mean first ionization potential (scaled on Carbon atom)
11	GD	graph density
12	nAT	number of atoms
13	nSK	number of non-H atoms
14	nAA	number of aromatic atoms
15	nTA	number of terminal atoms
16	nBT	number of bonds
17	nBO	number of non-H bonds
18	nBM	number of multiple bonds
19	SCBO	sum of conventional bond orders (H-depleted)
20	RBN	number of rotatable bonds
21	RBF	rotatable bond fraction
22	nDB	number of double bonds
23	nTB	number of triple bonds
24	nAB	number of aromatic bonds
25	nH	number of Hydrogen atoms
26	nC	number of Carbon atoms
27	nN	number of Nitrogen atoms
28	nO	number of Oxygen atoms
29	nP	number of Phosphorous atoms
30	nS	number of Sulfur atoms
31	nF	number of Fluorine atoms
32	nCL	number of Chlorine atoms
33	nBR	number of Bromine atoms
34	nI	number of Iodine atoms
35	nB	number of Boron atoms
36	nHM	number of heavy atoms
37	nHet	number of heteroatoms
38	nX	number of halogen atoms
39	H%	percentage of H atoms

40	C%	percentage of C atoms
41	N%	percentage of N atoms
42	O%	percentage of O atoms
43	X%	percentage of halogen atoms
44	nCsp3	number of sp3 hybridized Carbon atoms
45	nCsp2	number of sp2 hybridized Carbon atoms
46	nCsp	number of sp hybridized Carbon atoms
47	Fsp3	number of sp3 hybridized carbons/total carbon count
48	max_conj_path	maximum number of atoms that can be in conjugation with each other
49	nStructures	number of disconnected structures
50	totalcharge	total charge

2. Ring descriptors

No.	Name	Description
51	nCIC	number of rings (cyclomatic number)
52	nCIR	number of circuits
53	TRS	total ring size
54	Rperim	ring perimeter
55	Rbrid	ring bridge count
56	MCD	molecular cyclized degree
57	RFD	ring fusion density
58	RCI	ring complexity index
59	NRS	number of ring systems
60	NNRS	normalized number of ring systems
61	nSpiro	number of spiro atoms
62	nBridgeHead	number of bridgehead atoms
63	nR03	number of 3-membered rings
64	nR04	number of 4-membered rings
65	nR05	number of 5-membered rings
66	nR06	number of 6-membered rings
67	nR07	number of 7-membered rings
68	nR08	number of 8-membered rings
69	nR09	number of 9-membered rings
70	nR10	number of 10-membered rings
71	nR11	number of 11-membered rings
72	nR12	number of 12-membered rings
73	nBnz	number of benzene-like rings
74	ARR	aromatic ratio
75	AP	aromatic proportion
76	D/Dtr03	distance/detour ring index of order 3
77	D/Dtr04	distance/detour ring index of order 4
78	D/Dtr05	distance/detour ring index of order 5

79	D/Dtr06	distance/detour ring index of order 6
80	D/Dtr07	distance/detour ring index of order 7
81	D/Dtr08	distance/detour ring index of order 8
82	D/Dtr09	distance/detour ring index of order 9
83	D/Dtr10	distance/detour ring index of order 10
84	D/Dtr11	distance/detour ring index of order 11
85	D/Dtr12	distance/detour ring index of order 12

3. Topological indices

No.	Name	Description
86	ZM1	first Zagreb index
87	ZM1V	first Zagreb index by valence vertex degrees
88	ZM1Kup	first Zagreb index by Kupchik vertex degrees
89	ZM1Mad	first Zagreb index by Madan vertex degrees
90	ZM1Per	first Zagreb index by perturbation vertex degrees
91	ZM1MulPer	first Zagreb index by multiplicative perturbation vertex degrees
92	ZM2	second Zagreb index
93	ZM2V	second Zagreb index by valence vertex degrees
94	ZM2Kup	second Zagreb index by Kupchik vertex degrees
95	ZM2Mad	second Zagreb index by Madan vertex degrees
96	ZM2Per	second Zagreb index by perturbation vertex degrees
97	ZM2MulPer	second Zagreb index by multiplicative perturbation vertex degrees
98	ON0	overall modified Zagreb index of order 0
99	ON0V	overall modified Zagreb index of order 0 by valence vertex degrees
100	ON1	overall modified Zagreb index of order 1
101	ON1V	overall modified Zagreb index of order 1 by valence vertex degrees
102	Qindex	quadratic index
103	BBI	Bertz branching index
104	DBI	Dragon branching index
105	SNar	Narumi simple topological index (log function)
106	HNar	Narumi harmonic topological index
107	GNar	Narumi geometric topological index
108	Xt	total structure connectivity index
109	Dz	Pogliani index
110	Ram	ramification index
111	BLI	Kier benzene-likeliness index
112	Pol	polarity number
113	LPRS	log of product of row sums (PRS)
114	MSD	mean square distance index (Balaban)
115	SPI	superpendentic index
116	PJI2	2D Petitjean shape index
117	ECC	eccentricity

118	AECC	average eccentricity
119	DECC	eccentric
120	MDDD	mean distance degree deviation
121	UNIP	unipolarity
122	CENT	centralization
123	VAR	variation
124	ICR	radial centric information index
125	MaxTD	max topological distance
126	MeanTD	mean pairwise topological distance
127	MaxDD	max detour distance
128	MeanDD	mean pairwise detour distance
129	SMTI	Schultz Molecular Topological Index (MTI)
130	SMTIV	Schultz Molecular Topological Index by valence vertex degrees
131	GMTI	Gutman Molecular Topological Index
132	GMTIV	Gutman Molecular Topological Index by valence vertex degrees
133	Xu	Xu index
134	CSI	eccentric connectivity index
135	Wap	all-path Wiener index
136	S1K	1-path Kier alpha-modified shape index
137	S2K	2-path Kier alpha-modified shape index
138	S3K	3-path Kier alpha-modified shape index
139	PHI	Kier flexibility index
140	PW2	path/walk 2 – Randic shape index
141	PW3	path/walk 3 – Randic shape index
142	PW4	path/walk 4 – Randic shape index
143	PW5	path/walk 5 – Randic shape index
144	MAXDN	maximal electrotopological negative variation
145	MAXDP	maximal electrotopological positive variation
146	DELS	molecular electrotopological variation
147	TIE	E-state topological parameter
148	Psi_i_s	intrinsic state pseudoconnectivity index – type S
149	Psi_i_A	intrinsic state pseudoconnectivity index – type S average
150	Psi_i_0	intrinsic state pseudoconnectivity index – type 0
151	Psi_i_1	intrinsic state pseudoconnectivity index – type 1
152	Psi_i_t	intrinsic state pseudoconnectivity index – type T
153	Psi_i_0d	intrinsic state pseudoconnectivity index – type 0d
154	Psi_i_1d	intrinsic state pseudoconnectivity index – type 1d
155	Psi_i_1s	intrinsic state pseudoconnectivity index – type 1s
156	Psi_e_A	electrotopological state pseudoconnectivity index – type S average
157	Psi_e_0	electrotopological state pseudoconnectivity index – type 0
158	Psi_e_1	electrotopological state pseudoconnectivity index – type 1
159	Psi_e_t	electrotopological state pseudoconnectivity index – type T

160	Psi_e_0d	electrotopological state pseudoconnectivity index – type 0d
161	Psi_e_1d	electrotopological state pseudoconnectivity index – type 1d
162	Psi_e_1s	electrotopological state pseudoconnectivity index – type 1s
163	BAC	Balaban centric index
164	LOC	lopping centric index

4. Walk and path counts

No.	Name	Description
165	MWC01	molecular walk count of order 1
166	MWC02	molecular walk count of order 2
167	MWC03	molecular walk count of order 3
168	MWC04	molecular walk count of order 4
169	MWC05	molecular walk count of order 5
170	MWC06	molecular walk count of order 6
171	MWC07	molecular walk count of order 7
172	MWC08	molecular walk count of order 8
173	MWC09	molecular walk count of order 9
174	MWC10	molecular walk count of order 10
175	SRW02	self-returning walk count of order 2
176	SRW03	self-returning walk count of order 3
177	SRW04	self-returning walk count of order 4
178	SRW05	self-returning walk count of order 5
179	SRW06	self-returning walk count of order 6
180	SRW07	self-returning walk count of order 7
181	SRW08	self-returning walk count of order 8
182	SRW09	self-returning walk count of order 9
183	SRW10	self-returning walk count of order 10
184	MPC01	molecular path count of order 1 (no. of non-H bonds)
185	MPC02	molecular path count of order 2 (Gordon-Scantlebury index)
186	MPC03	molecular path count of order 3
187	MPC04	molecular path count of order 4
188	MPC05	molecular path count of order 5
189	MPC06	molecular path count of order 6
190	MPC07	molecular path count of order 7
191	MPC08	molecular path count of order 8
192	MPC09	molecular path count of order 9
193	MPC10	molecular path count of order 10
194	piPC01	molecular multiple path count of order 1
195	piPC02	molecular multiple path count of order 2
196	piPC03	molecular multiple path count of order 3
197	piPC04	molecular multiple path count of order 4
198	piPC05	molecular multiple path count of order 5

199	piPC06	molecular multiple path count of order 6
200	piPC07	molecular multiple path count of order 7
201	piPC08	molecular multiple path count of order 8
202	piPC09	molecular multiple path count of order 9
203	piPC10	molecular multiple path count of order 10
204	TWC	total walk count
205	TPC	total path count
206	piID	conventional bond order ID number
207	PCR	ratio of multiple path count over path count
208	PCD	difference between multiple path count and path count
209	CID	Randic ID number
210	BID	Balaban ID number

5. Connectivity indices

No.	Name	Description
211	X0	connectivity index of order 0
212	X1	connectivity index of order 1 (Randic connectivity index)
213	X2	connectivity index of order 2
214	X3	connectivity index of order 3
215	X4	connectivity index of order 4
216	X5	connectivity index of order 5
217	X0A	average connectivity index of order 0
218	X1A	average connectivity index of order 1
219	X2A	average connectivity index of order 2
220	X3A	average connectivity index of order 3
221	X4A	average connectivity index of order 4
222	X5A	average connectivity index of order 5
223	X0v	valence connectivity index of order 0
224	X1v	valence connectivity index of order 1
225	X2v	valence connectivity index of order 2
226	X3v	valence connectivity index of order 3
227	X4v	valence connectivity index of order 4
228	X5v	valence connectivity index of order 5
229	X0Av	average valence connectivity index of order 0
230	X1Av	average valence connectivity index of order 1
231	X2Av	average valence connectivity index of order 2
232	X3Av	average valence connectivity index of order 3
233	X4Av	average valence connectivity index of order 4
234	X5Av	average valence connectivity index of order 5
235	X0sol	solvation connectivity index of order 0
236	X1sol	solvation connectivity index of order 1
237	X2sol	solvation connectivity index of order 2

238	X3sol	solvation connectivity index of order 3
239	X4sol	solvation connectivity index of order 4
240	X5sol	solvation connectivity index of order 5
241	XMOD	modified Randic index
242	RDCHI	reciprocal distance sum Randic-like index
243	RDSQ	reciprocal distance sum inverse Randic-like index
244	X1Kup	Kupchik connectivity index
245	X1Mad	connectivity topochemical index
246	X1Per	perturbation connectivity index
247	X1MulPer	multiplicative perturbation connectivity index

6. Information indices

No.	Name	Description
248	ISIZ	information index on molecular size
249	IAC	total information index on atomic composition
250	AAC	mean information index on atomic composition
251	IDE	mean information content on the distance equality
252	IDM	mean information content on the distance magnitude
253	IDDE	mean information content on the distance degree equality
254	IDDM	mean information content on the distance degree magnitude
255	IDET	total information content on the distance equality
256	IDMT	total information content on the distance magnitude
257	IVDE	mean information content on the vertex degree equality
258	IVDM	mean information content on the vertex degree magnitude
259	Ges	Number of symmetry classes (based on electrotopological state)
260	rGes	Relative number of symmetry classes (based on electrotopological state)
261	S0K	Kier symmetry index
262	HVcpx	graph vertex complexity index
263	HDcpx	graph distance complexity index (log function)
264	Uindex	Balaban U index
265	Vindex	Balaban V index
266	Xindex	Balaban X index
267	Yindex	Balaban Y index
268	BertzCT	Bertz complexity index
269	IC0	Information Content index (neighborhood symmetry of 0-order)
270	IC1	Information Content index (neighborhood symmetry of 1-order)
271	IC2	Information Content index (neighborhood symmetry of 2-order)
272	IC3	Information Content index (neighborhood symmetry of 3-order)
273	IC4	Information Content index (neighborhood symmetry of 4-order)
274	IC5	Information Content index (neighborhood symmetry of 5-order)
275	TIC0	Total Information Content index (neighborhood symmetry of 0-order)
276	TIC1	Total Information Content index (neighborhood symmetry of 1-order)

277	TIC2	Total Information Content index (neighborhood symmetry of 2-order)
278	TIC3	Total Information Content index (neighborhood symmetry of 3-order)
279	TIC4	Total Information Content index (neighborhood symmetry of 4-order)
280	TIC5	Total Information Content index (neighborhood symmetry of 5-order)
281	SIC0	Structural Information Content index (neighborhood symmetry of 0-order)
282	SIC1	Structural Information Content index (neighborhood symmetry of 1-order)
283	SIC2	Structural Information Content index (neighborhood symmetry of 2-order)
284	SIC3	Structural Information Content index (neighborhood symmetry of 3-order)
285	SIC4	Structural Information Content index (neighborhood symmetry of 4-order)
286	SIC5	Structural Information Content index (neighborhood symmetry of 5-order)
287	CIC0	Complementary Information Content index (neighborhood symmetry of 0-order)
288	CIC1	Complementary Information Content index (neighborhood symmetry of 1-order)
289	CIC2	Complementary Information Content index (neighborhood symmetry of 2-order)
290	CIC3	Complementary Information Content index (neighborhood symmetry of 3-order)
291	CIC4	Complementary Information Content index (neighborhood symmetry of 4-order)
292	CIC5	Complementary Information Content index (neighborhood symmetry of 5-order)
293	BIC0	Bond Information Content index (neighborhood symmetry of 0-order)
294	BIC1	Bond Information Content index (neighborhood symmetry of 1-order)
295	BIC2	Bond Information Content index (neighborhood symmetry of 2-order)
296	BIC3	Bond Information Content index (neighborhood symmetry of 3-order)
297	BIC4	Bond Information Content index (neighborhood symmetry of 4-order)
298	BIC5	Bond Information Content index (neighborhood symmetry of 5-order)

7. 2D matrix-based descriptors

No.	Name	Description
299	J_A	Balaban-like index from adjacency matrix
300	SpPos_A	spectral positive sum from adjacency matrix
301	SpPosA_A	normalized spectral positive sum from adjacency matrix
302	SpPosLog_A	logarithmic spectral positive sum from adjacency matrix
303	SpMax_A	leading eigenvalue from adjacency matrix (Lovasz-Pelikan index)
304	SpMaxA_A	normalized leading eigenvalue from adjacency matrix
305	SpDiam_A	spectral diameter from adjacency matrix
306	SpAD_A	spectral absolute deviation from adjacency matrix
307	SpMAD_A	spectral mean absolute deviation from adjacency matrix
308	Ho_A	Hosoya-like index (log function) from adjacency matrix
309	EE_A	Estrada-like index (log function) from adjacency matrix
310	VE1_A	coefficient sum of the last eigenvector (absolute values) from adjacency matrix
311	VE2_A	average coefficient of the last eigenvector (absolute values) from adjacency matrix
312	VE3_A	logarithmic coefficient sum of the last eigenvector (absolute values) from adjacency matrix
313	VE1sign_A	coefficient sum of the last eigenvector from adjacency matrix
314	VE2sign_A	average coefficient of the last eigenvector from adjacency matrix
315	VE3sign_A	logarithmic coefficient sum of the last eigenvector from adjacency matrix

316	VR1_A	Randic-like eigenvector-based index from adjacency matrix
317	VR2_A	normalized Randic-like eigenvector-based index from adjacency matrix
318	VR3_A	logarithmic Randic-like eigenvector-based index from adjacency matrix
319	Wi_D	Wiener-like index from topological distance matrix (Wiener index)
320	WiA_D	average Wiener-like index from topological distance matrix
321	AVS_D	average vertex sum from topological distance matrix
322	H_D	Harary-like index from topological distance matrix (Harary index)
323	Chi_D	Randic-like index from topological distance matrix
324	ChiA_D	average Randic-like index from topological distance matrix
325	J_D	Balaban-like index from topological distance matrix (Balaban distance connectivity index)
326	HyWi_D	hyper-Wiener-like index (log function) from topological distance matrix
327	SpPos_D	spectral positive sum from topological distance matrix
328	SpPosA_D	normalized spectral positive sum from topological distance matrix
329	SpPosLog_D	logarithmic spectral positive sum from topological distance matrix
330	SpMax_D	leading eigenvalue from topological distance matrix
331	SpMaxA_D	normalized leading eigenvalue from topological distance matrix
332	SpDiam_D	spectral diameter from topological distance matrix
333	SpAD_D	spectral absolute deviation from topological distance matrix
334	SpMAD_D	spectral mean absolute deviation from topological distance matrix
335	Ho_D	Hosoya-like index (log function) from topological distance matrix
336	EE_D	Estrada-like index (log function) from topological distance matrix
337	SM2_D	spectral moment of order 2 from topological distance matrix
338	SM3_D	spectral moment of order 3 from topological distance matrix
339	SM4_D	spectral moment of order 4 from topological distance matrix
340	SM5_D	spectral moment of order 5 from topological distance matrix
341	SM6_D	spectral moment of order 6 from topological distance matrix
342	VE1_D	coefficient sum of the last eigenvector (absolute values) from topological distance matrix
343	VE2_D	average coefficient of the last eigenvector (absolute values) from topological distance matrix
344	VE3_D	logarithmic coefficient sum of the last eigenvector (absolute values) from topological distance matrix
345	VE1sign_D	coefficient sum of the last eigenvector from topological distance matrix
346	VE2sign_D	average coefficient of the last eigenvector from topological distance matrix
347	VE3sign_D	logarithmic coefficient sum of the last eigenvector from topological distance matrix
348	VR1_D	Randic-like eigenvector-based index from topological distance matrix
349	VR2_D	normalized Randic-like eigenvector-based index from topological distance matrix
350	VR3_D	logarithmic Randic-like eigenvector-based index from topological distance matrix
351	Acon	algebraic connectivity (also known as Fiedler value or Fiedler eigenvalue)
352	QW_L	quasi-Wiener index (Kirchhoff number) from Laplace matrix
353	TI1_L	first Mohar index from Laplace matrix
354	TI2_L	second Mohar index from Laplace matrix
355	STN_L	spanning tree number (log function) from Laplace matrix
356	SpPos_L	spectral positive sum from Laplace matrix
357	SpPosA_L	normalized spectral positive sum from Laplace matrix

358	SpPosLog_L	logarithmic spectral positive sum from Laplace matrix
359	SpMax_L	leading eigenvalue from Laplace matrix
360	SpMaxA_L	normalized leading eigenvalue from Laplace matrix
361	SpDiam_L	spectral diameter from Laplace matrix
362	SpAD_L	spectral absolute deviation from Laplace matrix
363	SpMAD_L	spectral mean absolute deviation from Laplace matrix
364	Ho_L	Hosoya-like index (log function) from Laplace matrix
365	EE_L	Estrada-like index (log function) from Laplace matrix
366	SM2_L	spectral moment of order 2 from Laplace matrix
367	SM3_L	spectral moment of order 3 from Laplace matrix
368	SM4_L	spectral moment of order 4 from Laplace matrix
369	SM5_L	spectral moment of order 5 from Laplace matrix
370	SM6_L	spectral moment of order 6 from Laplace matrix
371	VE1_L	coefficient sum of the last eigenvector (absolute values) from Laplace matrix
372	VE2_L	average coefficient of the last eigenvector (absolute values) from Laplace matrix
373	VE3_L	logarithmic coefficient sum of the last eigenvector (absolute values) from Laplace matrix
374	VE1sign_L	coefficient sum of the last eigenvector from Laplace matrix
375	VE2sign_L	average coefficient of the last eigenvector from Laplace matrix
376	VE3sign_L	logarithmic coefficient sum of the last eigenvector from Laplace matrix
377	VR1_L	Randic-like eigenvector-based index from Laplace matrix
378	VR2_L	normalized Randic-like eigenvector-based index from Laplace matrix
379	VR3_L	logarithmic Randic-like eigenvector-based index from Laplace matrix
380	AVS_X	average vertex sum from chi matrix
381	H_X	Harary-like index from chi matrix
382	Chi_X	Randic-like index from chi matrix
383	ChiA_X	average Randic-like index from chi matrix
384	J_X	Balaban-like index from chi matrix
385	HyWi_X	hyper-Wiener-like index (log function) from chi matrix
386	SpPos_X	spectral positive sum from chi matrix
387	SpPosA_X	normalized spectral positive sum from chi matrix
388	SpPosLog_X	logarithmic spectral positive sum from chi matrix
389	SpMax_X	leading eigenvalue from chi matrix
390	SpMaxA_X	normalized leading eigenvalue from chi matrix
391	SpDiam_X	spectral diameter from chi matrix
392	SpAD_X	spectral absolute deviation from chi matrix
393	SpMAD_X	spectral mean absolute deviation from chi matrix
394	Ho_X	Hosoya-like index (log function) from chi matrix
395	EE_X	Estrada-like index (log function) from chi matrix
396	SM2_X	spectral moment of order 2 from chi matrix
397	SM3_X	spectral moment of order 3 from chi matrix
398	SM4_X	spectral moment of order 4 from chi matrix
399	SM5_X	spectral moment of order 5 from chi matrix

400	SM6_X	spectral moment of order 6 from chi matrix
401	VE1_X	coefficient sum of the last eigenvector (absolute values) from chi matrix
402	VE2_X	average coefficient of the last eigenvector (absolute values) from chi matrix
403	VE3_X	logarithmic coefficient sum of the last eigenvector (absolute values) from chi matrix
404	VE1sign_X	coefficient sum of the last eigenvector from chi matrix
405	VE2sign_X	average coefficient of the last eigenvector from chi matrix
406	VE3sign_X	logarithmic coefficient sum of the last eigenvector from chi matrix
407	VR1_X	Randic-like eigenvector-based index from chi matrix
408	VR2_X	normalized Randic-like eigenvector-based index from chi matrix
409	VR3_X	logarithmic Randic-like eigenvector-based index from chi matrix
410	Wi_H2	Wiener-like index from reciprocal squared distance matrix
411	WiA_H2	average Wiener-like index from reciprocal squared distance matrix
412	AVS_H2	average vertex sum from reciprocal squared distance matrix
413	Chi_H2	Randic-like index from reciprocal squared distance matrix
414	ChiA_H2	average Randic-like index from reciprocal squared distance matrix
415	J_H2	Balaban-like index from reciprocal squared distance matrix
416	HyWi_H2	hyper-Wiener-like index (log function) from reciprocal squared distance matrix
417	SpPos_H2	spectral positive sum from reciprocal squared distance matrix
418	SpPosA_H2	normalized spectral positive sum from reciprocal squared distance matrix
419	SpPosLog_H2	logarithmic spectral positive sum from reciprocal squared distance matrix
420	SpMax_H2	leading eigenvalue from reciprocal squared distance matrix
421	SpMaxA_H2	normalized leading eigenvalue from reciprocal squared distance matrix
422	SpDiam_H2	spectral diameter from reciprocal squared distance matrix
423	SpAD_H2	spectral absolute deviation from reciprocal squared distance matrix
424	SpMAD_H2	spectral mean absolute deviation from reciprocal squared distance matrix
425	Ho_H2	Hosoya-like index (log function) from reciprocal squared distance matrix
426	EE_H2	Estrada-like index (log function) from reciprocal squared distance matrix
427	SM2_H2	spectral moment of order 2 from reciprocal squared distance matrix
428	SM3_H2	spectral moment of order 3 from reciprocal squared distance matrix
429	SM4_H2	spectral moment of order 4 from reciprocal squared distance matrix
430	SM5_H2	spectral moment of order 5 from reciprocal squared distance matrix
431	SM6_H2	spectral moment of order 6 from reciprocal squared distance matrix
432	VE1_H2	coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix
433	VE2_H2	average coefficient of the last eigenvector (absolute values) from reciprocal squared distance matrix
434	VE3_H2	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix
435	VE1sign_H2	coefficient sum of the last eigenvector from reciprocal squared distance matrix
436	VE2sign_H2	average coefficient of the last eigenvector from reciprocal squared distance matrix
437	VE3sign_H2	logarithmic coefficient sum of the last eigenvector from reciprocal squared distance matrix
438	VR1_H2	Randic-like eigenvector-based index from reciprocal squared distance matrix
439	VR2_H2	normalized Randic-like eigenvector-based index from reciprocal squared distance matrix
440	VR3_H2	logarithmic Randic-like eigenvector-based index from reciprocal squared distance matrix
441	Wi_Dt	Wiener-like index from detour matrix (detour index)

442	WiA_Dt	average Wiener-like index from detour matrix
443	AVS_Dt	average vertex sum from detour matrix
444	H_Dt	Harary-like index from detour matrix
445	Chi_Dt	Randic-like index from detour matrix
446	ChiA_Dt	average Randic-like index from detour matrix
447	J_Dt	Balaban-like index from detour matrix
448	HyWi_Dt	hyper-Wiener-like index (log function) from detour matrix
449	SpPos_Dt	spectral positive sum from detour matrix
450	SpPosA_Dt	normalized spectral positive sum from detour matrix
451	SpPosLog_Dt	logarithmic spectral positive sum from detour matrix
452	SpMax_Dt	leading eigenvalue from detour matrix
453	SpMaxA_Dt	normalized leading eigenvalue from detour matrix
454	SpDiam_Dt	spectral diameter from detour matrix
455	SpAD_Dt	spectral absolute deviation from detour matrix
456	SpMAD_Dt	spectral mean absolute deviation from detour matrix
457	Ho_Dt	Hosoya-like index (log function) from detour matrix
458	EE_Dt	Estrada-like index (log function) from detour matrix
459	SM2_Dt	spectral moment of order 2 from detour matrix
460	SM3_Dt	spectral moment of order 3 from detour matrix
461	SM4_Dt	spectral moment of order 4 from detour matrix
462	SM5_Dt	spectral moment of order 5 from detour matrix
463	SM6_Dt	spectral moment of order 6 from detour matrix
464	VE1_Dt	coefficient sum of the last eigenvector (absolute values) from detour matrix
465	VE2_Dt	average coefficient of the last eigenvector (absolute values) from detour matrix
466	VE3_Dt	logarithmic coefficient sum of the last eigenvector (absolute values) from detour matrix
467	VE1sign_Dt	coefficient sum of the last eigenvector from detour matrix
468	VE2sign_Dt	average coefficient of the last eigenvector from detour matrix
469	VE3sign_Dt	logarithmic coefficient sum of the last eigenvector from detour matrix
470	VR1_Dt	Randic-like eigenvector-based index from detour matrix
471	VR2_Dt	normalized Randic-like eigenvector-based index from detour matrix
472	VR3_Dt	logarithmic Randic-like eigenvector-based index from detour matrix
473	Wi_D/Dt	Wiener-like index from distance/detour matrix
474	WiA_D/Dt	average Wiener-like index from distance/detour matrix
475	AVS_D/Dt	average vertex sum from distance/detour matrix
476	H_D/Dt	Harary-like index from distance/detour matrix
477	Chi_D/Dt	Randic-like index from distance/detour matrix
478	ChiA_D/Dt	average Randic-like index from distance/detour matrix
479	J_D/Dt	Balaban-like index from distance/detour matrix
480	HyWi_D/Dt	hyper-Wiener-like index (log function) from distance/detour matrix
481	SpPos_D/Dt	spectral positive sum from distance/detour matrix
482	SpPosA_D/Dt	normalized spectral positive sum from distance/detour matrix
483	SpPosLog_D/Dt	logarithmic spectral positive sum from distance/detour matrix

484	SpMax_D/Dt	leading eigenvalue from distance/detour matrix
485	SpMaxA_D/Dt	normalized leading eigenvalue from distance/detour matrix
486	SpDiam_D/Dt	spectral diameter from distance/detour matrix
487	SpAD_D/Dt	spectral absolute deviation from distance/detour matrix
488	SpMAD_D/Dt	spectral mean absolute deviation from distance/detour matrix
489	Ho_D/Dt	Hosoya-like index (log function) from distance/detour matrix
490	EE_D/Dt	Estrada-like index (log function) from distance/detour matrix
491	SM2_D/Dt	spectral moment of order 2 from distance/detour matrix
492	SM3_D/Dt	spectral moment of order 3 from distance/detour matrix
493	SM4_D/Dt	spectral moment of order 4 from distance/detour matrix
494	SM5_D/Dt	spectral moment of order 5 from distance/detour matrix
495	SM6_D/Dt	spectral moment of order 6 from distance/detour matrix
496	VE1_D/Dt	coefficient sum of the last eigenvector (absolute values) from distance/detour matrix
497	VE2_D/Dt	average coefficient of the last eigenvector (absolute values) from distance/detour matrix
498	VE3_D/Dt	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/detour matrix
499	VE1sign_D/Dt	coefficient sum of the last eigenvector from distance/detour matrix
500	VE2sign_D/Dt	average coefficient of the last eigenvector from distance/detour matrix
501	VE3sign_D/Dt	logarithmic coefficient sum of the last eigenvector from distance/detour matrix
502	VR1_D/Dt	Randic-like eigenvector-based index from distance/detour matrix
503	VR2_D/Dt	normalized Randic-like eigenvector-based index from distance/detour matrix
504	VR3_D/Dt	logarithmic Randic-like eigenvector-based index from distance/detour matrix
505	Wi_Dz(Z)	Wiener-like index from Barysz matrix weighted by atomic number
506	WiA_Dz(Z)	average Wiener-like index from Barysz matrix weighted by atomic number
507	AVS_Dz(Z)	average vertex sum from Barysz matrix weighted by atomic number
508	H_Dz(Z)	Harary-like index from Barysz matrix weighted by atomic number
509	Chi_Dz(Z)	Randic-like index from Barysz matrix weighted by atomic number
510	ChiA_Dz(Z)	average Randic-like index from Barysz matrix weighted by atomic number
511	J_Dz(Z)	Balaban-like index from Barysz matrix weighted by atomic number
512	HyWi_Dz(Z)	hyper-Wiener-like index (log function) from Barysz matrix weighted by atomic number
513	SpAbs_Dz(Z)	graph energy from Barysz matrix weighted by atomic number
514	SpPos_Dz(Z)	spectral positive sum from Barysz matrix weighted by atomic number
515	SpPosA_Dz(Z)	normalized spectral positive sum from Barysz matrix weighted by atomic number
516	SpPosLog_Dz(Z)	logarithmic spectral positive sum from Barysz matrix weighted by atomic number
517	SpMax_Dz(Z)	leading eigenvalue from Barysz matrix weighted by atomic number
518	SpMaxA_Dz(Z)	normalized leading eigenvalue from Barysz matrix weighted by atomic number
519	SpDiam_Dz(Z)	spectral diameter from Barysz matrix weighted by atomic number
520	SpAD_Dz(Z)	spectral absolute deviation from Barysz matrix weighted by atomic number
521	SpMAD_Dz(Z)	spectral mean absolute deviation from Barysz matrix weighted by atomic number
522	Ho_Dz(Z)	Hosoya-like index (log function) from Barysz matrix weighted by atomic number
523	EE_Dz(Z)	Estrada-like index (log function) from Barysz matrix weighted by atomic number
524	SM1_Dz(Z)	spectral moment of order 1 from Barysz matrix weighted by atomic number
525	SM2_Dz(Z)	spectral moment of order 2 from Barysz matrix weighted by atomic number

526	SM3_Dz(Z)	spectral moment of order 3 from Barysz matrix weighted by atomic number
527	SM4_Dz(Z)	spectral moment of order 4 from Barysz matrix weighted by atomic number
528	SM5_Dz(Z)	spectral moment of order 5 from Barysz matrix weighted by atomic number
529	SM6_Dz(Z)	spectral moment of order 6 from Barysz matrix weighted by atomic number
530	VE1_Dz(Z)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number
531	VE2_Dz(Z)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number
532	VE3_Dz(Z)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number
533	VE1sign_Dz(Z)	coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number
534	VE2sign_Dz(Z)	average coefficient of the last eigenvector from Barysz matrix weighted by atomic number
535	VE3sign_Dz(Z)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number
536	VR1_Dz(Z)	Randic-like eigenvector-based index from Barysz matrix weighted by atomic number
537	VR2_Dz(Z)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by atomic number
538	VR3_Dz(Z)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by atomic number
539	Wi_Dz(m)	Wiener-like index from Barysz matrix weighted by mass
540	WiA_Dz(m)	average Wiener-like index from Barysz matrix weighted by mass
541	AVS_Dz(m)	average vertex sum from Barysz matrix weighted by mass
542	H_Dz(m)	Harary-like index from Barysz matrix weighted by mass
543	Chi_Dz(m)	Randic-like index from Barysz matrix weighted by mass
544	ChiA_Dz(m)	average Randic-like index from Barysz matrix weighted by mass
545	J_Dz(m)	Balaban-like index from Barysz matrix weighted by mass
546	HyWi_Dz(m)	hyper-Wiener-like index (log function) from Barysz matrix weighted by mass
547	SpAbs_Dz(m)	graph energy from Barysz matrix weighted by mass
548	SpPos_Dz(m)	spectral positive sum from Barysz matrix weighted by mass
549	SpPosA_Dz(m)	normalized spectral positive sum from Barysz matrix weighted by mass
550	SpPosLog_Dz(m)	logarithmic spectral positive sum from Barysz matrix weighted by mass
551	SpMax_Dz(m)	leading eigenvalue from Barysz matrix weighted by mass
552	SpMaxA_Dz(m)	normalized leading eigenvalue from Barysz matrix weighted by mass
553	SpDiam_Dz(m)	spectral diameter from Barysz matrix weighted by mass
554	SpAD_Dz(m)	spectral absolute deviation from Barysz matrix weighted by mass
555	SpMAD_Dz(m)	spectral mean absolute deviation from Barysz matrix weighted by mass
556	Ho_Dz(m)	Hosoya-like index (log function) from Barysz matrix weighted by mass
557	EE_Dz(m)	Estrada-like index (log function) from Barysz matrix weighted by mass
558	SM1_Dz(m)	spectral moment of order 1 from Barysz matrix weighted by mass
559	SM2_Dz(m)	spectral moment of order 2 from Barysz matrix weighted by mass
560	SM3_Dz(m)	spectral moment of order 3 from Barysz matrix weighted by mass
561	SM4_Dz(m)	spectral moment of order 4 from Barysz matrix weighted by mass
562	SM5_Dz(m)	spectral moment of order 5 from Barysz matrix weighted by mass
563	SM6_Dz(m)	spectral moment of order 6 from Barysz matrix weighted by mass
564	VE1_Dz(m)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass
565	VE2_Dz(m)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by mass
566	VE3_Dz(m)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass
567	VE1sign_Dz(m)	coefficient sum of the last eigenvector from Barysz matrix weighted by mass

568	VE2sign_Dz(m)	average coefficient of the last eigenvector from Barysz matrix weighted by mass
569	VE3sign_Dz(m)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by mass
570	VR1_Dz(m)	Randic-like eigenvector-based index from Barysz matrix weighted by mass
571	VR2_Dz(m)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by mass
572	VR3_Dz(m)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by mass
573	Wi_Dz(v)	Wiener-like index from Barysz matrix weighted by van der Waals volume
574	WiA_Dz(v)	average Wiener-like index from Barysz matrix weighted by van der Waals volume
575	AVS_Dz(v)	average vertex sum from Barysz matrix weighted by van der Waals volume
576	H_Dz(v)	Harary-like index from Barysz matrix weighted by van der Waals volume
577	Chi_Dz(v)	Randic-like index from Barysz matrix weighted by van der Waals volume
578	ChiA_Dz(v)	average Randic-like index from Barysz matrix weighted by van der Waals volume
579	J_Dz(v)	Balaban-like index from Barysz matrix weighted by van der Waals volume
580	HyWi_Dz(v)	hyper-Wiener-like index (log function) from Barysz matrix weighted by van der Waals volume
581	SpAbs_Dz(v)	graph energy from Barysz matrix weighted by van der Waals volume
582	SpPos_Dz(v)	spectral positive sum from Barysz matrix weighted by van der Waals volume
583	SpPosA_Dz(v)	normalized spectral positive sum from Barysz matrix weighted by van der Waals volume
584	SpPosLog_Dz(v)	logarithmic spectral positive sum from Barysz matrix weighted by van der Waals volume
585	SpMax_Dz(v)	leading eigenvalue from Barysz matrix weighted by van der Waals volume
586	SpMaxA_Dz(v)	normalized leading eigenvalue from Barysz matrix weighted by van der Waals volume
587	SpDiam_Dz(v)	spectral diameter from Barysz matrix weighted by van der Waals volume
588	SpAD_Dz(v)	spectral absolute deviation from Barysz matrix weighted by van der Waals volume
589	SpMAD_Dz(v)	spectral mean absolute deviation from Barysz matrix weighted by van der Waals volume
590	Ho_Dz(v)	Hosoya-like index (log function) from Barysz matrix weighted by van der Waals volume
591	EE_Dz(v)	Estrada-like index (log function) from Barysz matrix weighted by van der Waals volume
592	SM1_Dz(v)	spectral moment of order 1 from Barysz matrix weighted by van der Waals volume
593	SM2_Dz(v)	spectral moment of order 2 from Barysz matrix weighted by van der Waals volume
594	SM3_Dz(v)	spectral moment of order 3 from Barysz matrix weighted by van der Waals volume
595	SM4_Dz(v)	spectral moment of order 4 from Barysz matrix weighted by van der Waals volume
596	SM5_Dz(v)	spectral moment of order 5 from Barysz matrix weighted by van der Waals volume
597	SM6_Dz(v)	spectral moment of order 6 from Barysz matrix weighted by van der Waals volume
598	VE1_Dz(v)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume
599	VE2_Dz(v)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume
600	VE3_Dz(v)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume
601	VE1sign_Dz(v)	coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume
602	VE2sign_Dz(v)	average coefficient of the last eigenvector from Barysz matrix weighted by van der Waals volume
603	VE3sign_Dz(v)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume
604	VR1_Dz(v)	Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume
605	VR2_Dz(v)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume
606	VR3_Dz(v)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume
607	Wi_Dz(e)	Wiener-like index from Barysz matrix weighted by Sanderson electronegativity
608	WiA_Dz(e)	average Wiener-like index from Barysz matrix weighted by Sanderson electronegativity
609	AVS_Dz(e)	average vertex sum from Barysz matrix weighted by Sanderson electronegativity

610	H_Dz(e)	Harary-like index from Barysz matrix weighted by Sanderson electronegativity
611	Chi_Dz(e)	Randic-like index from Barysz matrix weighted by Sanderson electronegativity
612	ChiA_Dz(e)	average Randic-like index from Barysz matrix weighted by Sanderson electronegativity
613	J_Dz(e)	Balaban-like index from Barysz matrix weighted by Sanderson electronegativity
614	HyWi_Dz(e)	hyper-Wiener-like index (log function) from Barysz matrix weighted by Sanderson electronegativity
615	SpAbs_Dz(e)	graph energy from Barysz matrix weighted by Sanderson electronegativity
616	SpPos_Dz(e)	spectral positive sum from Barysz matrix weighted by Sanderson electronegativity
617	SpPosA_Dz(e)	normalized spectral positive sum from Barysz matrix weighted by Sanderson electronegativity
618	SpPosLog_Dz(e)	logarithmic spectral positive sum from Barysz matrix weighted by Sanderson electronegativity
619	SpMax_Dz(e)	leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity
620	SpMaxA_Dz(e)	normalized leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity
621	SpDiam_Dz(e)	spectral diameter from Barysz matrix weighted by Sanderson electronegativity
622	SpAD_Dz(e)	spectral absolute deviation from Barysz matrix weighted by Sanderson electronegativity
623	SpMAD_Dz(e)	spectral mean absolute deviation from Barysz matrix weighted by Sanderson electronegativity
624	Ho_Dz(e)	Hosoya-like index (log function) from Barysz matrix weighted by Sanderson electronegativity
625	EE_Dz(e)	Estrada-like index (log function) from Barysz matrix weighted by Sanderson electronegativity
626	SM1_Dz(e)	spectral moment of order 1 from Barysz matrix weighted by Sanderson electronegativity
627	SM2_Dz(e)	spectral moment of order 2 from Barysz matrix weighted by Sanderson electronegativity
628	SM3_Dz(e)	spectral moment of order 3 from Barysz matrix weighted by Sanderson electronegativity
629	SM4_Dz(e)	spectral moment of order 4 from Barysz matrix weighted by Sanderson electronegativity
630	SM5_Dz(e)	spectral moment of order 5 from Barysz matrix weighted by Sanderson electronegativity
631	SM6_Dz(e)	spectral moment of order 6 from Barysz matrix weighted by Sanderson electronegativity
632	VE1_Dz(e)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity
633	VE2_Dz(e)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity
634	VE3_Dz(e)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity
635	VE1sign_Dz(e)	coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity
636	VE2sign_Dz(e)	average coefficient of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity
637	VE3sign_Dz(e)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity
638	VR1_Dz(e)	Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity
639	VR2_Dz(e)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity
640	VR3_Dz(e)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity
641	Wi_Dz(p)	Wiener-like index from Barysz matrix weighted by polarizability
642	WiA_Dz(p)	average Wiener-like index from Barysz matrix weighted by polarizability
643	AVS_Dz(p)	average vertex sum from Barysz matrix weighted by polarizability
644	H_Dz(p)	Harary-like index from Barysz matrix weighted by polarizability
645	Chi_Dz(p)	Randic-like index from Barysz matrix weighted by polarizability
646	ChiA_Dz(p)	average Randic-like index from Barysz matrix weighted by polarizability
647	J_Dz(p)	Balaban-like index from Barysz matrix weighted by polarizability
648	HyWi_Dz(p)	hyper-Wiener-like index (log function) from Barysz matrix weighted by polarizability
649	SpAbs_Dz(p)	graph energy from Barysz matrix weighted by polarizability
650	SpPos_Dz(p)	spectral positive sum from Barysz matrix weighted by polarizability
651	SpPosA_Dz(p)	normalized spectral positive sum from Barysz matrix weighted by polarizability

652	SpPosLog_Dz(p)	logarithmic spectral positive sum from Barysz matrix weighted by polarizability
653	SpMax_Dz(p)	leading eigenvalue from Barysz matrix weighted by polarizability
654	SpMaxA_Dz(p)	normalized leading eigenvalue from Barysz matrix weighted by polarizability
655	SpDiam_Dz(p)	spectral diameter from Barysz matrix weighted by polarizability
656	SpAD_Dz(p)	spectral absolute deviation from Barysz matrix weighted by polarizability
657	SpMAD_Dz(p)	spectral mean absolute deviation from Barysz matrix weighted by polarizability
658	Ho_Dz(p)	Hosoya-like index (log function) from Barysz matrix weighted by polarizability
659	EE_Dz(p)	Estrada-like index (log function) from Barysz matrix weighted by polarizability
660	SM1_Dz(p)	spectral moment of order 1 from Barysz matrix weighted by polarizability
661	SM2_Dz(p)	spectral moment of order 2 from Barysz matrix weighted by polarizability
662	SM3_Dz(p)	spectral moment of order 3 from Barysz matrix weighted by polarizability
663	SM4_Dz(p)	spectral moment of order 4 from Barysz matrix weighted by polarizability
664	SM5_Dz(p)	spectral moment of order 5 from Barysz matrix weighted by polarizability
665	SM6_Dz(p)	spectral moment of order 6 from Barysz matrix weighted by polarizability
666	VE1_Dz(p)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability
667	VE2_Dz(p)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability
668	VE3_Dz(p)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability
669	VE1sign_Dz(p)	coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability
670	VE2sign_Dz(p)	average coefficient of the last eigenvector from Barysz matrix weighted by polarizability
671	VE3sign_Dz(p)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability
672	VR1_Dz(p)	Randic-like eigenvector-based index from Barysz matrix weighted by polarizability
673	VR2_Dz(p)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by polarizability
674	VR3_Dz(p)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by polarizability
675	Wi_Dz(i)	Wiener-like index from Barysz matrix weighted by ionization potential
676	WiA_Dz(i)	average Wiener-like index from Barysz matrix weighted by ionization potential
677	AVS_Dz(i)	average vertex sum from Barysz matrix weighted by ionization potential
678	H_Dz(i)	Harary-like index from Barysz matrix weighted by ionization potential
679	Chi_Dz(i)	Randic-like index from Barysz matrix weighted by ionization potential
680	ChiA_Dz(i)	average Randic-like index from Barysz matrix weighted by ionization potential
681	J_Dz(i)	Balaban-like index from Barysz matrix weighted by ionization potential
682	HyWi_Dz(i)	hyper-Wiener-like index (log function) from Barysz matrix weighted by ionization potential
683	SpAbs_Dz(i)	graph energy from Barysz matrix weighted by ionization potential
684	SpPos_Dz(i)	spectral positive sum from Barysz matrix weighted by ionization potential
685	SpPosA_Dz(i)	normalized spectral positive sum from Barysz matrix weighted by ionization potential
686	SpPosLog_Dz(i)	logarithmic spectral positive sum from Barysz matrix weighted by ionization potential
687	SpMax_Dz(i)	leading eigenvalue from Barysz matrix weighted by ionization potential
688	SpMaxA_Dz(i)	normalized leading eigenvalue from Barysz matrix weighted by ionization potential
689	SpDiam_Dz(i)	spectral diameter from Barysz matrix weighted by ionization potential
690	SpAD_Dz(i)	spectral absolute deviation from Barysz matrix weighted by ionization potential
691	SpMAD_Dz(i)	spectral mean absolute deviation from Barysz matrix weighted by ionization potential
692	Ho_Dz(i)	Hosoya-like index (log function) from Barysz matrix weighted by ionization potential
693	EE_Dz(i)	Estrada-like index (log function) from Barysz matrix weighted by ionization potential

694	SM1_Dz(i)	spectral moment of order 1 from Barysz matrix weighted by ionization potential
695	SM2_Dz(i)	spectral moment of order 2 from Barysz matrix weighted by ionization potential
696	SM3_Dz(i)	spectral moment of order 3 from Barysz matrix weighted by ionization potential
697	SM4_Dz(i)	spectral moment of order 4 from Barysz matrix weighted by ionization potential
698	SM5_Dz(i)	spectral moment of order 5 from Barysz matrix weighted by ionization potential
699	SM6_Dz(i)	spectral moment of order 6 from Barysz matrix weighted by ionization potential
700	VE1_Dz(i)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential
701	VE2_Dz(i)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential
702	VE3_Dz(i)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential
703	VE1sign_Dz(i)	coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential
704	VE2sign_Dz(i)	average coefficient of the last eigenvector from Barysz matrix weighted by ionization potential
705	VE3sign_Dz(i)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential
706	VR1_Dz(i)	Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
707	VR2_Dz(i)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
708	VR3_Dz(i)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential
709	Wi_B(m)	Wiener-like index from Burden matrix weighted by mass
710	WiA_B(m)	average Wiener-like index from Burden matrix weighted by mass
711	AVS_B(m)	average vertex sum from Burden matrix weighted by mass
712	Chi_B(m)	Randic-like index from Burden matrix weighted by mass
713	ChiA_B(m)	average Randic-like index from Burden matrix weighted by mass
714	J_B(m)	Balaban-like index from Burden matrix weighted by mass
715	HyWi_B(m)	hyper-Wiener-like index (log function) from Burden matrix weighted by mass
716	SpAbs_B(m)	graph energy from Burden matrix weighted by mass
717	SpPos_B(m)	spectral positive sum from Burden matrix weighted by mass
718	SpPosA_B(m)	normalized spectral positive sum from Burden matrix weighted by mass
719	SpPosLog_B(m)	logarithmic spectral positive sum from Burden matrix weighted by mass
720	SpMax_B(m)	leading eigenvalue from Burden matrix weighted by mass
721	SpMaxA_B(m)	normalized leading eigenvalue from Burden matrix weighted by mass
722	SpDiam_B(m)	spectral diameter from Burden matrix weighted by mass
723	SpAD_B(m)	spectral absolute deviation from Burden matrix weighted by mass
724	SpMAD_B(m)	spectral mean absolute deviation from Burden matrix weighted by mass
725	Ho_B(m)	Hosoya-like index (log function) from Burden matrix weighted by mass
726	EE_B(m)	Estrada-like index (log function) from Burden matrix weighted by mass
727	SM1_B(m)	spectral moment of order 1 from Burden matrix weighted by mass
728	SM2_B(m)	spectral moment of order 2 from Burden matrix weighted by mass
729	SM3_B(m)	spectral moment of order 3 from Burden matrix weighted by mass
730	SM4_B(m)	spectral moment of order 4 from Burden matrix weighted by mass
731	SM5_B(m)	spectral moment of order 5 from Burden matrix weighted by mass
732	SM6_B(m)	spectral moment of order 6 from Burden matrix weighted by mass
733	VE1_B(m)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass
734	VE2_B(m)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by mass
735	VE3_B(m)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass

736	VE1sign_B(m)	coefficient sum of the last eigenvector from Burden matrix weighted by mass
737	VE2sign_B(m)	average coefficient of the last eigenvector from Burden matrix weighted by mass
738	VE3sign_B(m)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by mass
739	VR1_B(m)	Randic-like eigenvector-based index from Burden matrix weighted by mass
740	VR2_B(m)	normalized Randic-like eigenvector-based index from Burden matrix weighted by mass
741	VR3_B(m)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by mass
742	Wi_B(v)	Wiener-like index from Burden matrix weighted by van der Waals volume
743	WiA_B(v)	average Wiener-like index from Burden matrix weighted by van der Waals volume
744	AVS_B(v)	average vertex sum from Burden matrix weighted by van der Waals volume
745	Chi_B(v)	Randic-like index from Burden matrix weighted by van der Waals volume
746	ChiA_B(v)	average Randic-like index from Burden matrix weighted by van der Waals volume
747	J_B(v)	Balaban-like index from Burden matrix weighted by van der Waals volume
748	HyWi_B(v)	hyper-Wiener-like index (log function) from Burden matrix weighted by van der Waals volume
749	SpAbs_B(v)	graph energy from Burden matrix weighted by van der Waals volume
750	SpPos_B(v)	spectral positive sum from Burden matrix weighted by van der Waals volume
751	SpPosA_B(v)	normalized spectral positive sum from Burden matrix weighted by van der Waals volume
752	SpPosLog_B(v)	logarithmic spectral positive sum from Burden matrix weighted by van der Waals volume
753	SpMax_B(v)	leading eigenvalue from Burden matrix weighted by van der Waals volume
754	SpMaxA_B(v)	normalized leading eigenvalue from Burden matrix weighted by van der Waals volume
755	SpDiam_B(v)	spectral diameter from Burden matrix weighted by van der Waals volume
756	SpAD_B(v)	spectral absolute deviation from Burden matrix weighted by van der Waals volume
757	SpMAD_B(v)	spectral mean absolute deviation from Burden matrix weighted by van der Waals volume
758	Ho_B(v)	Hosoya-like index (log function) from Burden matrix weighted by van der Waals volume
759	EE_B(v)	Estrada-like index (log function) from Burden matrix weighted by van der Waals volume
760	SM1_B(v)	spectral moment of order 1 from Burden matrix weighted by van der Waals volume
761	SM2_B(v)	spectral moment of order 2 from Burden matrix weighted by van der Waals volume
762	SM3_B(v)	spectral moment of order 3 from Burden matrix weighted by van der Waals volume
763	SM4_B(v)	spectral moment of order 4 from Burden matrix weighted by van der Waals volume
764	SM5_B(v)	spectral moment of order 5 from Burden matrix weighted by van der Waals volume
765	SM6_B(v)	spectral moment of order 6 from Burden matrix weighted by van der Waals volume
766	VE1_B(v)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume
767	VE2_B(v)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume
768	VE3_B(v)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume
769	VE1sign_B(v)	coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume
770	VE2sign_B(v)	average coefficient of the last eigenvector from Burden matrix weighted by van der Waals volume
771	VE3sign_B(v)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume
772	VR1_B(v)	Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume
773	VR2_B(v)	normalized Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume
774	VR3_B(v)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume
775	Wi_B(e)	Wiener-like index from Burden matrix weighted by Sanderson electronegativity
776	WiA_B(e)	average Wiener-like index from Burden matrix weighted by Sanderson electronegativity
777	AVS_B(e)	average vertex sum from Burden matrix weighted by Sanderson electronegativity

778	Chi_B(e)	Randic-like index from Burden matrix weighted by Sanderson electronegativity
779	ChiA_B(e)	average Randic-like index from Burden matrix weighted by Sanderson electronegativity
780	J_B(e)	Balaban-like index from Burden matrix weighted by Sanderson electronegativity
781	HyWi_B(e)	hyper-Wiener-like index (log function) from Burden matrix weighted by Sanderson electronegativity
782	SpAbs_B(e)	graph energy from Burden matrix weighted by Sanderson electronegativity
783	SpPos_B(e)	spectral positive sum from Burden matrix weighted by Sanderson electronegativity
784	SpPosA_B(e)	normalized spectral positive sum from Burden matrix weighted by Sanderson electronegativity
785	SpPosLog_B(e)	logarithmic spectral positive sum from Burden matrix weighted by Sanderson electronegativity
786	SpMax_B(e)	leading eigenvalue from Burden matrix weighted by Sanderson electronegativity
787	SpMaxA_B(e)	normalized leading eigenvalue from Burden matrix weighted by Sanderson electronegativity
788	SpDiam_B(e)	spectral diameter from Burden matrix weighted by Sanderson electronegativity
789	SpAD_B(e)	spectral absolute deviation from Burden matrix weighted by Sanderson electronegativity
790	SpMAD_B(e)	spectral mean absolute deviation from Burden matrix weighted by Sanderson electronegativity
791	Ho_B(e)	Hosoya-like index (log function) from Burden matrix weighted by Sanderson electronegativity
792	EE_B(e)	Estrada-like index (log function) from Burden matrix weighted by Sanderson electronegativity
793	SM1_B(e)	spectral moment of order 1 from Burden matrix weighted by Sanderson electronegativity
794	SM2_B(e)	spectral moment of order 2 from Burden matrix weighted by Sanderson electronegativity
795	SM3_B(e)	spectral moment of order 3 from Burden matrix weighted by Sanderson electronegativity
796	SM4_B(e)	spectral moment of order 4 from Burden matrix weighted by Sanderson electronegativity
797	SM5_B(e)	spectral moment of order 5 from Burden matrix weighted by Sanderson electronegativity
798	SM6_B(e)	spectral moment of order 6 from Burden matrix weighted by Sanderson electronegativity
799	VE1_B(e)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity
800	VE2_B(e)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity
801	VE3_B(e)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity
802	VE1sign_B(e)	coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity
803	VE2sign_B(e)	average coefficient of the last eigenvector from Burden matrix weighted by Sanderson electronegativity
804	VE3sign_B(e)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity
805	VR1_B(e)	Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity
806	VR2_B(e)	normalized Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity
807	VR3_B(e)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity
808	Wi_B(p)	Wiener-like index from Burden matrix weighted by polarizability
809	WiA_B(p)	average Wiener-like index from Burden matrix weighted by polarizability
810	AVS_B(p)	average vertex sum from Burden matrix weighted by polarizability
811	Chi_B(p)	Randic-like index from Burden matrix weighted by polarizability
812	ChiA_B(p)	average Randic-like index from Burden matrix weighted by polarizability
813	J_B(p)	Balaban-like index from Burden matrix weighted by polarizability
814	HyWi_B(p)	hyper-Wiener-like index (log function) from Burden matrix weighted by polarizability
815	SpAbs_B(p)	graph energy from Burden matrix weighted by polarizability
816	SpPos_B(p)	spectral positive sum from Burden matrix weighted by polarizability
817	SpPosA_B(p)	normalized spectral positive sum from Burden matrix weighted by polarizability
818	SpPosLog_B(p)	logarithmic spectral positive sum from Burden matrix weighted by polarizability
819	SpMax_B(p)	leading eigenvalue from Burden matrix weighted by polarizability

820	SpMaxA_B(p)	normalized leading eigenvalue from Burden matrix weighted by polarizability
821	SpDiam_B(p)	spectral diameter from Burden matrix weighted by polarizability
822	SpAD_B(p)	spectral absolute deviation from Burden matrix weighted by polarizability
823	SpMAD_B(p)	spectral mean absolute deviation from Burden matrix weighted by polarizability
824	Ho_B(p)	Hosoya-like index (log function) from Burden matrix weighted by polarizability
825	EE_B(p)	Estrada-like index (log function) from Burden matrix weighted by polarizability
826	SM1_B(p)	spectral moment of order 1 from Burden matrix weighted by polarizability
827	SM2_B(p)	spectral moment of order 2 from Burden matrix weighted by polarizability
828	SM3_B(p)	spectral moment of order 3 from Burden matrix weighted by polarizability
829	SM4_B(p)	spectral moment of order 4 from Burden matrix weighted by polarizability
830	SM5_B(p)	spectral moment of order 5 from Burden matrix weighted by polarizability
831	SM6_B(p)	spectral moment of order 6 from Burden matrix weighted by polarizability
832	VE1_B(p)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability
833	VE2_B(p)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by polarizability
834	VE3_B(p)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability
835	VE1sign_B(p)	coefficient sum of the last eigenvector from Burden matrix weighted by polarizability
836	VE2sign_B(p)	average coefficient of the last eigenvector from Burden matrix weighted by polarizability
837	VE3sign_B(p)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by polarizability
838	VR1_B(p)	Randic-like eigenvector-based index from Burden matrix weighted by polarizability
839	VR2_B(p)	normalized Randic-like eigenvector-based index from Burden matrix weighted by polarizability
840	VR3_B(p)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by polarizability
841	Wi_B(i)	Wiener-like index from Burden matrix weighted by ionization potential
842	WiA_B(i)	average Wiener-like index from Burden matrix weighted by ionization potential
843	AVS_B(i)	average vertex sum from Burden matrix weighted by ionization potential
844	Chi_B(i)	Randic-like index from Burden matrix weighted by ionization potential
845	ChiA_B(i)	average Randic-like index from Burden matrix weighted by ionization potential
846	J_B(i)	Balaban-like index from Burden matrix weighted by ionization potential
847	HyWi_B(i)	hyper-Wiener-like index (log function) from Burden matrix weighted by ionization potential
848	SpAbs_B(i)	graph energy from Burden matrix weighted by ionization potential
849	SpPos_B(i)	spectral positive sum from Burden matrix weighted by ionization potential
850	SpPosA_B(i)	normalized spectral positive sum from Burden matrix weighted by ionization potential
851	SpPosLog_B(i)	logarithmic spectral positive sum from Burden matrix weighted by ionization potential
852	SpMax_B(i)	leading eigenvalue from Burden matrix weighted by ionization potential
853	SpMaxA_B(i)	normalized leading eigenvalue from Burden matrix weighted by ionization potential
854	SpDiam_B(i)	spectral diameter from Burden matrix weighted by ionization potential
855	SpAD_B(i)	spectral absolute deviation from Burden matrix weighted by ionization potential
856	SpMAD_B(i)	spectral mean absolute deviation from Burden matrix weighted by ionization potential
857	Ho_B(i)	Hosoya-like index (log function) from Burden matrix weighted by ionization potential
858	EE_B(i)	Estrada-like index (log function) from Burden matrix weighted by ionization potential
859	SM1_B(i)	spectral moment of order 1 from Burden matrix weighted by ionization potential
860	SM2_B(i)	spectral moment of order 2 from Burden matrix weighted by ionization potential
861	SM3_B(i)	spectral moment of order 3 from Burden matrix weighted by ionization potential

862	SM4_B(i)	spectral moment of order 4 from Burden matrix weighted by ionization potential
863	SM5_B(i)	spectral moment of order 5 from Burden matrix weighted by ionization potential
864	SM6_B(i)	spectral moment of order 6 from Burden matrix weighted by ionization potential
865	VE1_B(i)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential
866	VE2_B(i)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential
867	VE3_B(i)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential
868	VE1sign_B(i)	coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential
869	VE2sign_B(i)	average coefficient of the last eigenvector from Burden matrix weighted by ionization potential
870	VE3sign_B(i)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential
871	VR1_B(i)	Randic-like eigenvector-based index from Burden matrix weighted by ionization potential
872	VR2_B(i)	normalized Randic-like eigenvector-based index from Burden matrix weighted by ionization potential
873	VR3_B(i)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by ionization potential
874	Wi_B(s)	Wiener-like index from Burden matrix weighted by I-State
875	WiA_B(s)	average Wiener-like index from Burden matrix weighted by I-State
876	AVS_B(s)	average vertex sum from Burden matrix weighted by I-State
877	Chi_B(s)	Randic-like index from Burden matrix weighted by I-State
878	ChiA_B(s)	average Randic-like index from Burden matrix weighted by I-State
879	J_B(s)	Balaban-like index from Burden matrix weighted by I-State
880	HyWi_B(s)	hyper-Wiener-like index (log function) from Burden matrix weighted by I-State
881	SpAbs_B(s)	graph energy from Burden matrix weighted by I-State
882	SpPos_B(s)	spectral positive sum from Burden matrix weighted by I-State
883	SpPosA_B(s)	normalized spectral positive sum from Burden matrix weighted by I-State
884	SpPosLog_B(s)	logarithmic spectral positive sum from Burden matrix weighted by I-State
885	SpMax_B(s)	leading eigenvalue from Burden matrix weighted by I-State
886	SpMaxA_B(s)	normalized leading eigenvalue from Burden matrix weighted by I-State
887	SpDiam_B(s)	spectral diameter from Burden matrix weighted by I-State
888	SpAD_B(s)	spectral absolute deviation from Burden matrix weighted by I-State
889	SpMAD_B(s)	spectral mean absolute deviation from Burden matrix weighted by I-State
890	Ho_B(s)	Hosoya-like index (log function) from Burden matrix weighted by I-State
891	EE_B(s)	Estrada-like index (log function) from Burden matrix weighted by I-State
892	SM1_B(s)	spectral moment of order 1 from Burden matrix weighted by I-State
893	SM2_B(s)	spectral moment of order 2 from Burden matrix weighted by I-State
894	SM3_B(s)	spectral moment of order 3 from Burden matrix weighted by I-State
895	SM4_B(s)	spectral moment of order 4 from Burden matrix weighted by I-State
896	SM5_B(s)	spectral moment of order 5 from Burden matrix weighted by I-State
897	SM6_B(s)	spectral moment of order 6 from Burden matrix weighted by I-State
898	VE1_B(s)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State
899	VE2_B(s)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by I-State
900	VE3_B(s)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State
901	VE1sign_B(s)	coefficient sum of the last eigenvector from Burden matrix weighted by I-State
902	VE2sign_B(s)	average coefficient of the last eigenvector from Burden matrix weighted by I-State
903	VE3sign_B(s)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by I-State

904	VR1_B(s)	Randic-like eigenvector-based index from Burden matrix weighted by I-State
905	VR2_B(s)	normalized Randic-like eigenvector-based index from Burden matrix weighted by I-State
906	VR3_B(s)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by I-State

8. 2D autocorrelations

No.	Name	Description
907	ATS1m	Broto-Moreau autocorrelation of lag 1 (log function) weighted by mass
908	ATS2m	Broto-Moreau autocorrelation of lag 2 (log function) weighted by mass
909	ATS3m	Broto-Moreau autocorrelation of lag 3 (log function) weighted by mass
910	ATS4m	Broto-Moreau autocorrelation of lag 4 (log function) weighted by mass
911	ATS5m	Broto-Moreau autocorrelation of lag 5 (log function) weighted by mass
912	ATS6m	Broto-Moreau autocorrelation of lag 6 (log function) weighted by mass
913	ATS7m	Broto-Moreau autocorrelation of lag 7 (log function) weighted by mass
914	ATS8m	Broto-Moreau autocorrelation of lag 8 (log function) weighted by mass
915	ATS1v	Broto-Moreau autocorrelation of lag 1 (log function) weighted by van der Waals volume
916	ATS2v	Broto-Moreau autocorrelation of lag 2 (log function) weighted by van der Waals volume
917	ATS3v	Broto-Moreau autocorrelation of lag 3 (log function) weighted by van der Waals volume
918	ATS4v	Broto-Moreau autocorrelation of lag 4 (log function) weighted by van der Waals volume
919	ATS5v	Broto-Moreau autocorrelation of lag 5 (log function) weighted by van der Waals volume
920	ATS6v	Broto-Moreau autocorrelation of lag 6 (log function) weighted by van der Waals volume
921	ATS7v	Broto-Moreau autocorrelation of lag 7 (log function) weighted by van der Waals volume
922	ATS8v	Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume
923	ATS1e	Broto-Moreau autocorrelation of lag 1 (log function) weighted by Sanderson electronegativity
924	ATS2e	Broto-Moreau autocorrelation of lag 2 (log function) weighted by Sanderson electronegativity
925	ATS3e	Broto-Moreau autocorrelation of lag 3 (log function) weighted by Sanderson electronegativity
926	ATS4e	Broto-Moreau autocorrelation of lag 4 (log function) weighted by Sanderson electronegativity
927	ATS5e	Broto-Moreau autocorrelation of lag 5 (log function) weighted by Sanderson electronegativity
928	ATS6e	Broto-Moreau autocorrelation of lag 6 (log function) weighted by Sanderson electronegativity
929	ATS7e	Broto-Moreau autocorrelation of lag 7 (log function) weighted by Sanderson electronegativity
930	ATS8e	Broto-Moreau autocorrelation of lag 8 (log function) weighted by Sanderson electronegativity
931	ATS1p	Broto-Moreau autocorrelation of lag 1 (log function) weighted by polarizability
932	ATS2p	Broto-Moreau autocorrelation of lag 2 (log function) weighted by polarizability
933	ATS3p	Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability
934	ATS4p	Broto-Moreau autocorrelation of lag 4 (log function) weighted by polarizability
935	ATS5p	Broto-Moreau autocorrelation of lag 5 (log function) weighted by polarizability
936	ATS6p	Broto-Moreau autocorrelation of lag 6 (log function) weighted by polarizability
937	ATS7p	Broto-Moreau autocorrelation of lag 7 (log function) weighted by polarizability
938	ATS8p	Broto-Moreau autocorrelation of lag 8 (log function) weighted by polarizability
939	ATS1i	Broto-Moreau autocorrelation of lag 1 (log function) weighted by ionization potential
940	ATS2i	Broto-Moreau autocorrelation of lag 2 (log function) weighted by ionization potential
941	ATS3i	Broto-Moreau autocorrelation of lag 3 (log function) weighted by ionization potential
942	ATS4i	Broto-Moreau autocorrelation of lag 4 (log function) weighted by ionization potential

943	ATS5i	Broto-Moreau autocorrelation of lag 5 (log function) weighted by ionization potential
944	ATS6i	Broto-Moreau autocorrelation of lag 6 (log function) weighted by ionization potential
945	ATS7i	Broto-Moreau autocorrelation of lag 7 (log function) weighted by ionization potential
946	ATS8i	Broto-Moreau autocorrelation of lag 8 (log function) weighted by ionization potential
947	ATS1s	Broto-Moreau autocorrelation of lag 1 (log function) weighted by I-state
948	ATS2s	Broto-Moreau autocorrelation of lag 2 (log function) weighted by I-state
949	ATS3s	Broto-Moreau autocorrelation of lag 3 (log function) weighted by I-state
950	ATS4s	Broto-Moreau autocorrelation of lag 4 (log function) weighted by I-state
951	ATS5s	Broto-Moreau autocorrelation of lag 5 (log function) weighted by I-state
952	ATS6s	Broto-Moreau autocorrelation of lag 6 (log function) weighted by I-state
953	ATS7s	Broto-Moreau autocorrelation of lag 7 (log function) weighted by I-state
954	ATS8s	Broto-Moreau autocorrelation of lag 8 (log function) weighted by I-state
955	ATSC1m	Centred Broto-Moreau autocorrelation of lag 1 weighted by mass
956	ATSC2m	Centred Broto-Moreau autocorrelation of lag 2 weighted by mass
957	ATSC3m	Centred Broto-Moreau autocorrelation of lag 3 weighted by mass
958	ATSC4m	Centred Broto-Moreau autocorrelation of lag 4 weighted by mass
959	ATSC5m	Centred Broto-Moreau autocorrelation of lag 5 weighted by mass
960	ATSC6m	Centred Broto-Moreau autocorrelation of lag 6 weighted by mass
961	ATSC7m	Centred Broto-Moreau autocorrelation of lag 7 weighted by mass
962	ATSC8m	Centred Broto-Moreau autocorrelation of lag 8 weighted by mass
963	ATSC1v	Centred Broto-Moreau autocorrelation of lag 1 weighted by van der Waals volume
964	ATSC2v	Centred Broto-Moreau autocorrelation of lag 2 weighted by van der Waals volume
965	ATSC3v	Centred Broto-Moreau autocorrelation of lag 3 weighted by van der Waals volume
966	ATSC4v	Centred Broto-Moreau autocorrelation of lag 4 weighted by van der Waals volume
967	ATSC5v	Centred Broto-Moreau autocorrelation of lag 5 weighted by van der Waals volume
968	ATSC6v	Centred Broto-Moreau autocorrelation of lag 6 weighted by van der Waals volume
969	ATSC7v	Centred Broto-Moreau autocorrelation of lag 7 weighted by van der Waals volume
970	ATSC8v	Centred Broto-Moreau autocorrelation of lag 8 weighted by van der Waals volume
971	ATSC1e	Centred Broto-Moreau autocorrelation of lag 1 weighted by Sanderson electronegativity
972	ATSC2e	Centred Broto-Moreau autocorrelation of lag 2 weighted by Sanderson electronegativity
973	ATSC3e	Centred Broto-Moreau autocorrelation of lag 3 weighted by Sanderson electronegativity
974	ATSC4e	Centred Broto-Moreau autocorrelation of lag 4 weighted by Sanderson electronegativity
975	ATSC5e	Centred Broto-Moreau autocorrelation of lag 5 weighted by Sanderson electronegativity
976	ATSC6e	Centred Broto-Moreau autocorrelation of lag 6 weighted by Sanderson electronegativity
977	ATSC7e	Centred Broto-Moreau autocorrelation of lag 7 weighted by Sanderson electronegativity
978	ATSC8e	Centred Broto-Moreau autocorrelation of lag 8 weighted by Sanderson electronegativity
979	ATSC1p	Centred Broto-Moreau autocorrelation of lag 1 weighted by polarizability
980	ATSC2p	Centred Broto-Moreau autocorrelation of lag 2 weighted by polarizability
981	ATSC3p	Centred Broto-Moreau autocorrelation of lag 3 weighted by polarizability
982	ATSC4p	Centred Broto-Moreau autocorrelation of lag 4 weighted by polarizability
983	ATSC5p	Centred Broto-Moreau autocorrelation of lag 5 weighted by polarizability
984	ATSC6p	Centred Broto-Moreau autocorrelation of lag 6 weighted by polarizability

985	ATSC7p	Centred Broto-Moreau autocorrelation of lag 7 weighted by polarizability
986	ATSC8p	Centred Broto-Moreau autocorrelation of lag 8 weighted by polarizability
987	ATSC1i	Centred Broto-Moreau autocorrelation of lag 1 weighted by ionization potential
988	ATSC2i	Centred Broto-Moreau autocorrelation of lag 2 weighted by ionization potential
989	ATSC3i	Centred Broto-Moreau autocorrelation of lag 3 weighted by ionization potential
990	ATSC4i	Centred Broto-Moreau autocorrelation of lag 4 weighted by ionization potential
991	ATSC5i	Centred Broto-Moreau autocorrelation of lag 5 weighted by ionization potential
992	ATSC6i	Centred Broto-Moreau autocorrelation of lag 6 weighted by ionization potential
993	ATSC7i	Centred Broto-Moreau autocorrelation of lag 7 weighted by ionization potential
994	ATSC8i	Centred Broto-Moreau autocorrelation of lag 8 weighted by ionization potential
995	ATSC1s	Centred Broto-Moreau autocorrelation of lag 1 weighted by I-state
996	ATSC2s	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state
997	ATSC3s	Centred Broto-Moreau autocorrelation of lag 3 weighted by I-state
998	ATSC4s	Centred Broto-Moreau autocorrelation of lag 4 weighted by I-state
999	ATSC5s	Centred Broto-Moreau autocorrelation of lag 5 weighted by I-state
1000	ATSC6s	Centred Broto-Moreau autocorrelation of lag 6 weighted by I-state
1001	ATSC7s	Centred Broto-Moreau autocorrelation of lag 7 weighted by I-state
1002	ATSC8s	Centred Broto-Moreau autocorrelation of lag 8 weighted by I-state
1003	MATS1m	Moran autocorrelation of lag 1 weighted by mass
1004	MATS2m	Moran autocorrelation of lag 2 weighted by mass
1005	MATS3m	Moran autocorrelation of lag 3 weighted by mass
1006	MATS4m	Moran autocorrelation of lag 4 weighted by mass
1007	MATS5m	Moran autocorrelation of lag 5 weighted by mass
1008	MATS6m	Moran autocorrelation of lag 6 weighted by mass
1009	MATS7m	Moran autocorrelation of lag 7 weighted by mass
1010	MATS8m	Moran autocorrelation of lag 8 weighted by mass
1011	MATS1v	Moran autocorrelation of lag 1 weighted by van der Waals volume
1012	MATS2v	Moran autocorrelation of lag 2 weighted by van der Waals volume
1013	MATS3v	Moran autocorrelation of lag 3 weighted by van der Waals volume
1014	MATS4v	Moran autocorrelation of lag 4 weighted by van der Waals volume
1015	MATS5v	Moran autocorrelation of lag 5 weighted by van der Waals volume
1016	MATS6v	Moran autocorrelation of lag 6 weighted by van der Waals volume
1017	MATS7v	Moran autocorrelation of lag 7 weighted by van der Waals volume
1018	MATS8v	Moran autocorrelation of lag 8 weighted by van der Waals volume
1019	MATS1e	Moran autocorrelation of lag 1 weighted by Sanderson electronegativity
1020	MATS2e	Moran autocorrelation of lag 2 weighted by Sanderson electronegativity
1021	MATS3e	Moran autocorrelation of lag 3 weighted by Sanderson electronegativity
1022	MATS4e	Moran autocorrelation of lag 4 weighted by Sanderson electronegativity
1023	MATS5e	Moran autocorrelation of lag 5 weighted by Sanderson electronegativity
1024	MATS6e	Moran autocorrelation of lag 6 weighted by Sanderson electronegativity
1025	MATS7e	Moran autocorrelation of lag 7 weighted by Sanderson electronegativity
1026	MATS8e	Moran autocorrelation of lag 8 weighted by Sanderson electronegativity

1027	MATS1p	Moran autocorrelation of lag 1 weighted by polarizability
1028	MATS2p	Moran autocorrelation of lag 2 weighted by polarizability
1029	MATS3p	Moran autocorrelation of lag 3 weighted by polarizability
1030	MATS4p	Moran autocorrelation of lag 4 weighted by polarizability
1031	MATS5p	Moran autocorrelation of lag 5 weighted by polarizability
1032	MATS6p	Moran autocorrelation of lag 6 weighted by polarizability
1033	MATS7p	Moran autocorrelation of lag 7 weighted by polarizability
1034	MATS8p	Moran autocorrelation of lag 8 weighted by polarizability
1035	MATS1i	Moran autocorrelation of lag 1 weighted by ionization potential
1036	MATS2i	Moran autocorrelation of lag 2 weighted by ionization potential
1037	MATS3i	Moran autocorrelation of lag 3 weighted by ionization potential
1038	MATS4i	Moran autocorrelation of lag 4 weighted by ionization potential
1039	MATS5i	Moran autocorrelation of lag 5 weighted by ionization potential
1040	MATS6i	Moran autocorrelation of lag 6 weighted by ionization potential
1041	MATS7i	Moran autocorrelation of lag 7 weighted by ionization potential
1042	MATS8i	Moran autocorrelation of lag 8 weighted by ionization potential
1043	MATS1s	Moran autocorrelation of lag 1 weighted by I-state
1044	MATS2s	Moran autocorrelation of lag 2 weighted by I-state
1045	MATS3s	Moran autocorrelation of lag 3 weighted by I-state
1046	MATS4s	Moran autocorrelation of lag 4 weighted by I-state
1047	MATS5s	Moran autocorrelation of lag 5 weighted by I-state
1048	MATS6s	Moran autocorrelation of lag 6 weighted by I-state
1049	MATS7s	Moran autocorrelation of lag 7 weighted by I-state
1050	MATS8s	Moran autocorrelation of lag 8 weighted by I-state
1051	GATS1m	Geary autocorrelation of lag 1 weighted by mass
1052	GATS2m	Geary autocorrelation of lag 2 weighted by mass
1053	GATS3m	Geary autocorrelation of lag 3 weighted by mass
1054	GATS4m	Geary autocorrelation of lag 4 weighted by mass
1055	GATS5m	Geary autocorrelation of lag 5 weighted by mass
1056	GATS6m	Geary autocorrelation of lag 6 weighted by mass
1057	GATS7m	Geary autocorrelation of lag 7 weighted by mass
1058	GATS8m	Geary autocorrelation of lag 8 weighted by mass
1059	GATS1v	Geary autocorrelation of lag 1 weighted by van der Waals volume
1060	GATS2v	Geary autocorrelation of lag 2 weighted by van der Waals volume
1061	GATS3v	Geary autocorrelation of lag 3 weighted by van der Waals volume
1062	GATS4v	Geary autocorrelation of lag 4 weighted by van der Waals volume
1063	GATS5v	Geary autocorrelation of lag 5 weighted by van der Waals volume
1064	GATS6v	Geary autocorrelation of lag 6 weighted by van der Waals volume
1065	GATS7v	Geary autocorrelation of lag 7 weighted by van der Waals volume
1066	GATS8v	Geary autocorrelation of lag 8 weighted by van der Waals volume
1067	GATS1e	Geary autocorrelation of lag 1 weighted by Sanderson electronegativity
1068	GATS2e	Geary autocorrelation of lag 2 weighted by Sanderson electronegativity

1069	GATS3e	Geary autocorrelation of lag 3 weighted by Sanderson electronegativity
1070	GATS4e	Geary autocorrelation of lag 4 weighted by Sanderson electronegativity
1071	GATS5e	Geary autocorrelation of lag 5 weighted by Sanderson electronegativity
1072	GATS6e	Geary autocorrelation of lag 6 weighted by Sanderson electronegativity
1073	GATS7e	Geary autocorrelation of lag 7 weighted by Sanderson electronegativity
1074	GATS8e	Geary autocorrelation of lag 8 weighted by Sanderson electronegativity
1075	GATS1p	Geary autocorrelation of lag 1 weighted by polarizability
1076	GATS2p	Geary autocorrelation of lag 2 weighted by polarizability
1077	GATS3p	Geary autocorrelation of lag 3 weighted by polarizability
1078	GATS4p	Geary autocorrelation of lag 4 weighted by polarizability
1079	GATS5p	Geary autocorrelation of lag 5 weighted by polarizability
1080	GATS6p	Geary autocorrelation of lag 6 weighted by polarizability
1081	GATS7p	Geary autocorrelation of lag 7 weighted by polarizability
1082	GATS8p	Geary autocorrelation of lag 8 weighted by polarizability
1083	GATS1i	Geary autocorrelation of lag 1 weighted by ionization potential
1084	GATS2i	Geary autocorrelation of lag 2 weighted by ionization potential
1085	GATS3i	Geary autocorrelation of lag 3 weighted by ionization potential
1086	GATS4i	Geary autocorrelation of lag 4 weighted by ionization potential
1087	GATS5i	Geary autocorrelation of lag 5 weighted by ionization potential
1088	GATS6i	Geary autocorrelation of lag 6 weighted by ionization potential
1089	GATS7i	Geary autocorrelation of lag 7 weighted by ionization potential
1090	GATS8i	Geary autocorrelation of lag 8 weighted by ionization potential
1091	GATS1s	Geary autocorrelation of lag 1 weighted by I-state
1092	GATS2s	Geary autocorrelation of lag 2 weighted by I-state
1093	GATS3s	Geary autocorrelation of lag 3 weighted by I-state
1094	GATS4s	Geary autocorrelation of lag 4 weighted by I-state
1095	GATS5s	Geary autocorrelation of lag 5 weighted by I-state
1096	GATS6s	Geary autocorrelation of lag 6 weighted by I-state
1097	GATS7s	Geary autocorrelation of lag 7 weighted by I-state
1098	GATS8s	Geary autocorrelation of lag 8 weighted by I-state
1099	GGI1	topological charge index of order 1
1100	GGI2	topological charge index of order 2
1101	GGI3	topological charge index of order 3
1102	GGI4	topological charge index of order 4
1103	GGI5	topological charge index of order 5
1104	GGI6	topological charge index of order 6
1105	GGI7	topological charge index of order 7
1106	GGI8	topological charge index of order 8
1107	GGI9	topological charge index of order 9
1108	GGI10	topological charge index of order 10
1109	JGI1	mean topological charge index of order 1
1110	JGI2	mean topological charge index of order 2

1111	JGI3	mean topological charge index of order 3
1112	JGI4	mean topological charge index of order 4
1113	JGI5	mean topological charge index of order 5
1114	JGI6	mean topological charge index of order 6
1115	JGI7	mean topological charge index of order 7
1116	JGI8	mean topological charge index of order 8
1117	JGI9	mean topological charge index of order 9
1118	JGI10	mean topological charge index of order 10
1119	JGT	global topological charge index

9. Burden eigenvalues

No.	Name	Description
1120	SpMax1_Bh(m)	largest eigenvalue n. 1 of Burden matrix weighted by mass
1121	SpMax2_Bh(m)	largest eigenvalue n. 2 of Burden matrix weighted by mass
1122	SpMax3_Bh(m)	largest eigenvalue n. 3 of Burden matrix weighted by mass
1123	SpMax4_Bh(m)	largest eigenvalue n. 4 of Burden matrix weighted by mass
1124	SpMax5_Bh(m)	largest eigenvalue n. 5 of Burden matrix weighted by mass
1125	SpMax6_Bh(m)	largest eigenvalue n. 6 of Burden matrix weighted by mass
1126	SpMax7_Bh(m)	largest eigenvalue n. 7 of Burden matrix weighted by mass
1127	SpMax8_Bh(m)	largest eigenvalue n. 8 of Burden matrix weighted by mass
1128	SpMax1_Bh(v)	largest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume
1129	SpMax2_Bh(v)	largest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume
1130	SpMax3_Bh(v)	largest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume
1131	SpMax4_Bh(v)	largest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume
1132	SpMax5_Bh(v)	largest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume
1133	SpMax6_Bh(v)	largest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume
1134	SpMax7_Bh(v)	largest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume
1135	SpMax8_Bh(v)	largest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume
1136	SpMax1_Bh(e)	largest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity
1137	SpMax2_Bh(e)	largest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity
1138	SpMax3_Bh(e)	largest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity
1139	SpMax4_Bh(e)	largest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity
1140	SpMax5_Bh(e)	largest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity
1141	SpMax6_Bh(e)	largest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity
1142	SpMax7_Bh(e)	largest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity
1143	SpMax8_Bh(e)	largest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity
1144	SpMax1_Bh(p)	largest eigenvalue n. 1 of Burden matrix weighted by polarizability
1145	SpMax2_Bh(p)	largest eigenvalue n. 2 of Burden matrix weighted by polarizability
1146	SpMax3_Bh(p)	largest eigenvalue n. 3 of Burden matrix weighted by polarizability
1147	SpMax4_Bh(p)	largest eigenvalue n. 4 of Burden matrix weighted by polarizability
1148	SpMax5_Bh(p)	largest eigenvalue n. 5 of Burden matrix weighted by polarizability
1149	SpMax6_Bh(p)	largest eigenvalue n. 6 of Burden matrix weighted by polarizability

1150	SpMax7_Bh(p)	largest eigenvalue n. 7 of Burden matrix weighted by polarizability
1151	SpMax8_Bh(p)	largest eigenvalue n. 8 of Burden matrix weighted by polarizability
1152	SpMax1_Bh(i)	largest eigenvalue n. 1 of Burden matrix weighted by ionization potential
1153	SpMax2_Bh(i)	largest eigenvalue n. 2 of Burden matrix weighted by ionization potential
1154	SpMax3_Bh(i)	largest eigenvalue n. 3 of Burden matrix weighted by ionization potential
1155	SpMax4_Bh(i)	largest eigenvalue n. 4 of Burden matrix weighted by ionization potential
1156	SpMax5_Bh(i)	largest eigenvalue n. 5 of Burden matrix weighted by ionization potential
1157	SpMax6_Bh(i)	largest eigenvalue n. 6 of Burden matrix weighted by ionization potential
1158	SpMax7_Bh(i)	largest eigenvalue n. 7 of Burden matrix weighted by ionization potential
1159	SpMax8_Bh(i)	largest eigenvalue n. 8 of Burden matrix weighted by ionization potential
1160	SpMax1_Bh(s)	largest eigenvalue n. 1 of Burden matrix weighted by I-state
1161	SpMax2_Bh(s)	largest eigenvalue n. 2 of Burden matrix weighted by I-state
1162	SpMax3_Bh(s)	largest eigenvalue n. 3 of Burden matrix weighted by I-state
1163	SpMax4_Bh(s)	largest eigenvalue n. 4 of Burden matrix weighted by I-state
1164	SpMax5_Bh(s)	largest eigenvalue n. 5 of Burden matrix weighted by I-state
1165	SpMax6_Bh(s)	largest eigenvalue n. 6 of Burden matrix weighted by I-state
1166	SpMax7_Bh(s)	largest eigenvalue n. 7 of Burden matrix weighted by I-state
1167	SpMax8_Bh(s)	largest eigenvalue n. 8 of Burden matrix weighted by I-state
1168	SpMin1_Bh(m)	smallest eigenvalue n. 1 of Burden matrix weighted by mass
1169	SpMin2_Bh(m)	smallest eigenvalue n. 2 of Burden matrix weighted by mass
1170	SpMin3_Bh(m)	smallest eigenvalue n. 3 of Burden matrix weighted by mass
1171	SpMin4_Bh(m)	smallest eigenvalue n. 4 of Burden matrix weighted by mass
1172	SpMin5_Bh(m)	smallest eigenvalue n. 5 of Burden matrix weighted by mass
1173	SpMin6_Bh(m)	smallest eigenvalue n. 6 of Burden matrix weighted by mass
1174	SpMin7_Bh(m)	smallest eigenvalue n. 7 of Burden matrix weighted by mass
1175	SpMin8_Bh(m)	smallest eigenvalue n. 8 of Burden matrix weighted by mass
1176	SpMin1_Bh(v)	smallest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume
1177	SpMin2_Bh(v)	smallest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume
1178	SpMin3_Bh(v)	smallest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume
1179	SpMin4_Bh(v)	smallest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume
1180	SpMin5_Bh(v)	smallest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume
1181	SpMin6_Bh(v)	smallest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume
1182	SpMin7_Bh(v)	smallest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume
1183	SpMin8_Bh(v)	smallest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume
1184	SpMin1_Bh(e)	smallest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity
1185	SpMin2_Bh(e)	smallest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity
1186	SpMin3_Bh(e)	smallest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity
1187	SpMin4_Bh(e)	smallest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity
1188	SpMin5_Bh(e)	smallest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity
1189	SpMin6_Bh(e)	smallest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity
1190	SpMin7_Bh(e)	smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity
1191	SpMin8_Bh(e)	smallest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity

1192	SpMin1_Bh(p)	smallest eigenvalue n. 1 of Burden matrix weighted by polarizability
1193	SpMin2_Bh(p)	smallest eigenvalue n. 2 of Burden matrix weighted by polarizability
1194	SpMin3_Bh(p)	smallest eigenvalue n. 3 of Burden matrix weighted by polarizability
1195	SpMin4_Bh(p)	smallest eigenvalue n. 4 of Burden matrix weighted by polarizability
1196	SpMin5_Bh(p)	smallest eigenvalue n. 5 of Burden matrix weighted by polarizability
1197	SpMin6_Bh(p)	smallest eigenvalue n. 6 of Burden matrix weighted by polarizability
1198	SpMin7_Bh(p)	smallest eigenvalue n. 7 of Burden matrix weighted by polarizability
1199	SpMin8_Bh(p)	smallest eigenvalue n. 8 of Burden matrix weighted by polarizability
1200	SpMin1_Bh(i)	smallest eigenvalue n. 1 of Burden matrix weighted by ionization potential
1201	SpMin2_Bh(i)	smallest eigenvalue n. 2 of Burden matrix weighted by ionization potential
1202	SpMin3_Bh(i)	smallest eigenvalue n. 3 of Burden matrix weighted by ionization potential
1203	SpMin4_Bh(i)	smallest eigenvalue n. 4 of Burden matrix weighted by ionization potential
1204	SpMin5_Bh(i)	smallest eigenvalue n. 5 of Burden matrix weighted by ionization potential
1205	SpMin6_Bh(i)	smallest eigenvalue n. 6 of Burden matrix weighted by ionization potential
1206	SpMin7_Bh(i)	smallest eigenvalue n. 7 of Burden matrix weighted by ionization potential
1207	SpMin8_Bh(i)	smallest eigenvalue n. 8 of Burden matrix weighted by ionization potential
1208	SpMin1_Bh(s)	smallest eigenvalue n. 1 of Burden matrix weighted by I-state
1209	SpMin2_Bh(s)	smallest eigenvalue n. 2 of Burden matrix weighted by I-state
1210	SpMin3_Bh(s)	smallest eigenvalue n. 3 of Burden matrix weighted by I-state
1211	SpMin4_Bh(s)	smallest eigenvalue n. 4 of Burden matrix weighted by I-state
1212	SpMin5_Bh(s)	smallest eigenvalue n. 5 of Burden matrix weighted by I-state
1213	SpMin6_Bh(s)	smallest eigenvalue n. 6 of Burden matrix weighted by I-state
1214	SpMin7_Bh(s)	smallest eigenvalue n. 7 of Burden matrix weighted by I-state
1215	SpMin8_Bh(s)	smallest eigenvalue n. 8 of Burden matrix weighted by I-state

10. P_VSA-like descriptors

No.	Name	Description
1216	P_VSA_LogP_1	P_VSA-like on LogP, bin 1
1217	P_VSA_LogP_2	P_VSA-like on LogP, bin 2
1218	P_VSA_LogP_3	P_VSA-like on LogP, bin 3
1219	P_VSA_LogP_4	P_VSA-like on LogP, bin 4
1220	P_VSA_LogP_5	P_VSA-like on LogP, bin 5
1221	P_VSA_LogP_6	P_VSA-like on LogP, bin 6
1222	P_VSA_LogP_7	P_VSA-like on LogP, bin 7
1223	P_VSA_LogP_8	P_VSA-like on LogP, bin 8
1224	P_VSA_MR_1	P_VSA-like on Molar Refractivity, bin 1
1225	P_VSA_MR_2	P_VSA-like on Molar Refractivity, bin 2
1226	P_VSA_MR_3	P_VSA-like on Molar Refractivity, bin 3
1227	P_VSA_MR_4	P_VSA-like on Molar Refractivity, bin 4
1228	P_VSA_MR_5	P_VSA-like on Molar Refractivity, bin 5
1229	P_VSA_MR_6	P_VSA-like on Molar Refractivity, bin 6
1230	P_VSA_MR_7	P_VSA-like on Molar Refractivity, bin 7

1231	P_VSA_MR_8	P_VSA-like on Molar Refractivity, bin 8
1232	P_VSA_m_1	P_VSA-like on mass, bin 1
1233	P_VSA_m_2	P_VSA-like on mass, bin 2
1234	P_VSA_m_3	P_VSA-like on mass, bin 3
1235	P_VSA_m_4	P_VSA-like on mass, bin 4
1236	P_VSA_m_5	P_VSA-like on mass, bin 5
1237	P_VSA_v_1	P_VSA-like on van der Waals volume, bin 1
1238	P_VSA_v_2	P_VSA-like on van der Waals volume, bin 2
1239	P_VSA_v_3	P_VSA-like on van der Waals volume, bin 3
1240	P_VSA_v_4	P_VSA-like on van der Waals volume, bin 4
1241	P_VSA_e_1	P_VSA-like on Sanderson electronegativity, bin 1
1242	P_VSA_e_2	P_VSA-like on Sanderson electronegativity, bin 2
1243	P_VSA_e_3	P_VSA-like on Sanderson electronegativity, bin 3
1244	P_VSA_e_4	P_VSA-like on Sanderson electronegativity, bin 4
1245	P_VSA_e_5	P_VSA-like on Sanderson electronegativity, bin 5
1246	P_VSA_e_6	P_VSA-like on Sanderson electronegativity, bin 6
1247	P_VSA_p_1	P_VSA-like on polarizability, bin 1
1248	P_VSA_p_2	P_VSA-like on polarizability, bin 2
1249	P_VSA_p_3	P_VSA-like on polarizability, bin 3
1250	P_VSA_p_4	P_VSA-like on polarizability, bin 4
1251	P_VSA_i_1	P_VSA-like on ionization potential, bin 1
1252	P_VSA_i_2	P_VSA-like on ionization potential, bin 2
1253	P_VSA_i_3	P_VSA-like on ionization potential, bin 3
1254	P_VSA_i_4	P_VSA-like on ionization potential, bin 4
1255	P_VSA_s_1	P_VSA-like on I-state, bin 1
1256	P_VSA_s_2	P_VSA-like on I-state, bin 2
1257	P_VSA_s_3	P_VSA-like on I-state, bin 3
1258	P_VSA_s_4	P_VSA-like on I-state, bin 4
1259	P_VSA_s_5	P_VSA-like on I-state, bin 5
1260	P_VSA_s_6	P_VSA-like on I-state, bin 6
1261	P_VSA_ppp_L	P_VSA-like on potential pharmacophore points, L – lipophilic
1262	P_VSA_ppp_P	P_VSA-like on potential pharmacophore points, P – positive
1263	P_VSA_ppp_N	P_VSA-like on potential pharmacophore points, N – negative
1264	P_VSA_ppp_D	P_VSA-like on potential pharmacophore points, D – hydrogen-bond donor
1265	P_VSA_ppp_A	P_VSA-like on potential pharmacophore points, A – hydrogen-bond acceptor
1266	P_VSA_ppp_ar	P_VSA-like on potential pharmacophore points, ar – aromatic atoms
1267	P_VSA_ppp_con	P_VSA-like on potential pharmacophore points, con – conjugated atoms
1268	P_VSA_ppp_hal	P_VSA-like on potential pharmacophore points, hal – halogen atoms
1269	P_VSA_ppp_cyc	P_VSA-like on potential pharmacophore points, cyc – atoms belonging to cycles
1270	P_VSA_ppp_ter	P_VSA-like on potential pharmacophore points, ter – terminal atoms
1271	P_VSA_charge_1	P_VSA-like on partial charges, bin 1
1272	P_VSA_charge_2	P_VSA-like on partial charges, bin 2

1273	P_VSA_charge_3	P_VSA-like on partial charges, bin 3
1274	P_VSA_charge_4	P_VSA-like on partial charges, bin 4
1275	P_VSA_charge_5	P_VSA-like on partial charges, bin 5
1276	P_VSA_charge_6	P_VSA-like on partial charges, bin 6
1277	P_VSA_charge_7	P_VSA-like on partial charges, bin 7
1278	P_VSA_charge_8	P_VSA-like on partial charges, bin 8
1279	P_VSA_charge_9	P_VSA-like on partial charges, bin 9
1280	P_VSA_charge_10	P_VSA-like on partial charges, bin 10
1281	P_VSA_charge_11	P_VSA-like on partial charges, bin 11
1282	P_VSA_charge_12	P_VSA-like on partial charges, bin 12
1283	P_VSA_charge_13	P_VSA-like on partial charges, bin 13
1284	P_VSA_charge_14	P_VSA-like on partial charges, bin 14

11. ETA indices

No.	Name	Description
1285	Eta_alpha	eta core count
1286	Eta_alpha_A	eta average core count
1287	Eta_epsi	eta electronegativity measure
1288	Eta_epsi_A	eta average electronegativity measure
1289	Eta_betaS	eta sigma VEM count
1290	Eta_betaS_A	eta sigma average VEM count
1291	Eta_betaP	eta pi and lone pair VEM count
1292	Eta_betaP_A	eta pi and lone pair average VEM count
1293	Eta_beta	eta VEM count
1294	Eta_beta_A	eta average VEM count
1295	Eta_C	eta composite index
1296	Eta_C_A	eta average composite index
1297	Eta_L	eta local composite index
1298	Eta_L_A	eta average local composite index
1299	Eta_R	eta composite index for reference alkane
1300	Eta_F	eta functionality index
1301	Eta_F_A	eta average functionality index
1302	Eta_LR	eta local composite index for reference alkane
1303	Eta_FL	eta local functionality index
1304	Eta_FL_A	eta average local functionality index
1305	Eta_B	eta branching index
1306	Eta_B_A	eta average branching index
1307	Eta_sh_p	eta p shape index
1308	Eta_sh_y	eta y shape index
1309	Eta_sh_x	eta x shape index
1310	Eta_D_AlphaA	eta delta alpha a index
1311	Eta_D_AlphaB	eta delta alpha b index

1312	Eta_epsi_2	eta electronegativity measure 2
1313	Eta_epsi_3	eta electronegativity measure 3
1314	Eta_epsi_4	eta electronegativity measure 4
1315	Eta_epsi_5	eta electronegativity measure 5
1316	Eta_D_epsiA	eta measure of unsaturation and electronegative atom count
1317	Eta_D_epsiB	eta measure of unsaturation
1318	Eta_D_epsiC	eta measure of electronegativity
1319	Eta_D_epsiD	eta measure of hydrogen bond donor atoms
1320	Eta_psi1	eta measure of hydrogen bonding propensity and/or polar surface area
1321	Eta_D_psiA	eta measure of hydrogen bonding propensity
1322	Eta_D_psiB	eta measure of hydrogen bonding propensity
1323	Eta_D_beta	eta measure of electronic features
1324	Eta_D_beta_A	eta average measure of electronic features

12. Edge adjacency indices

No.	Name	Description
1325	SpMax_EA	leading eigenvalue from edge adjacency mat.
1326	SpMaxA_EA	normalized leading eigenvalue from edge adjacency mat.
1327	SpDiam_EA	spectral diameter from edge adjacency mat.
1328	SpAD_EA	spectral absolute deviation from edge adjacency mat.
1329	SpMAD_EA	spectral mean absolute deviation from edge adjacency mat.
1330	SpMax_EA(ed)	leading eigenvalue from edge adjacency mat. weighted by edge degree
1331	SpMaxA_EA(ed)	normalized leading eigenvalue from edge adjacency mat. weighted by edge degree
1332	SpDiam_EA(ed)	spectral diameter from edge adjacency mat. weighted by edge degree
1333	SpAD_EA(ed)	spectral absolute deviation from edge adjacency mat. weighted by edge degree
1334	SpMAD_EA(ed)	spectral mean absolute deviation from edge adjacency mat. weighted by edge degree
1335	SpMax_EA(bo)	leading eigenvalue from edge adjacency mat. weighted by bond order
1336	SpMaxA_EA(bo)	normalized leading eigenvalue from edge adjacency mat. weighted by bond order
1337	SpDiam_EA(bo)	spectral diameter from edge adjacency mat. weighted by bond order
1338	SpAD_EA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order
1339	SpMAD_EA(bo)	spectral mean absolute deviation from edge adjacency mat. weighted by bond order
1340	SpMax_EA(dm)	leading eigenvalue from edge adjacency mat. weighted by dipole moment
1341	SpMaxA_EA(dm)	normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment
1342	SpDiam_EA(dm)	spectral diameter from edge adjacency mat. weighted by dipole moment
1343	SpAD_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by dipole moment
1344	SpMAD_EA(dm)	spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment
1345	SpMax_EA(ri)	leading eigenvalue from edge adjacency mat. weighted by resonance integral
1346	SpMaxA_EA(ri)	normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral
1347	SpDiam_EA(ri)	spectral diameter from edge adjacency mat. weighted by resonance integral
1348	SpAD_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by resonance integral
1349	SpMAD_EA(ri)	spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral
1350	SpMax_AEA(ed)	leading eigenvalue from augmented edge adjacency mat. weighted by edge degree

1351	SpMaxA_AEA(ed)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree
1352	SpDiam_AEA(ed)	spectral diameter from augmented edge adjacency mat. weighted by edge degree
1353	SpAD_AEA(ed)	spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree
1354	SpMAD_AEA(ed)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree
1355	SpMax_AEA(bo)	leading eigenvalue from augmented edge adjacency mat. weighted by bond order
1356	SpMaxA_AEA(bo)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order
1357	SpDiam_AEA(bo)	spectral diameter from augmented edge adjacency mat. weighted by bond order
1358	SpAD_AEA(bo)	spectral absolute deviation from augmented edge adjacency mat. weighted by bond order
1359	SpMAD_AEA(bo)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order
1360	SpMax_AEA(dm)	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment
1361	SpMaxA_AEA(dm)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment
1362	SpDiam_AEA(dm)	spectral diameter from augmented edge adjacency mat. weighted by dipole moment
1363	SpAD_AEA(dm)	spectral absolute deviation from augmented edge adjacency mat. weighted by dipole moment
1364	SpMAD_AEA(dm)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by dipole moment
1365	SpMax_AEA(ri)	leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral
1366	SpMaxA_AEA(ri)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral
1367	SpDiam_AEA(ri)	spectral diameter from augmented edge adjacency mat. weighted by resonance integral
1368	SpAD_AEA(ri)	spectral absolute deviation from augmented edge adjacency mat. weighted by resonance integral
1369	SpMAD_AEA(ri)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by resonance integral
1370	Chi0_EA	connectivity-like index of order 0 from edge adjacency mat.
1371	Chi1_EA	connectivity-like index of order 1 from edge adjacency mat.
1372	Chi0_EA(ed)	connectivity-like index of order 0 from edge adjacency mat. weighted by edge degree
1373	Chi1_EA(ed)	connectivity-like index of order 1 from edge adjacency mat. weighted by edge degree
1374	Chi0_EA(bo)	connectivity-like index of order 0 from edge adjacency mat. weighted by bond order
1375	Chi1_EA(bo)	connectivity-like index of order 1 from edge adjacency mat. weighted by bond order
1376	Chi0_EA(dm)	connectivity-like index of order 0 from edge adjacency mat. weighted by dipole moment
1377	Chi1_EA(dm)	connectivity-like index of order 1 from edge adjacency mat. weighted by dipole moment
1378	Chi0_EA(ri)	connectivity-like index of order 0 from edge adjacency mat. weighted by resonance integral
1379	Chi1_EA(ri)	connectivity-like index of order 1 from edge adjacency mat. weighted by resonance integral
1380	Chi0_AEA(ed)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by edge degree
1381	Chi1_AEA(ed)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by edge degree
1382	Chi0_AEA(bo)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by bond order
1383	Chi1_AEA(bo)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by bond order
1384	Chi0_AEA(dm)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by dipole moment
1385	Chi1_AEA(dm)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by dipole moment
1386	Chi0_AEA(ri)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by resonance integral
1387	Chi1_AEA(ri)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by resonance integral
1388	SM02_EA	spectral moment of order 2 from edge adjacency mat.
1389	SM03_EA	spectral moment of order 3 from edge adjacency mat.
1390	SM04_EA	spectral moment of order 4 from edge adjacency mat.
1391	SM05_EA	spectral moment of order 5 from edge adjacency mat.
1392	SM06_EA	spectral moment of order 6 from edge adjacency mat.

1393	SM07_EA	spectral moment of order 7 from edge adjacency mat.
1394	SM08_EA	spectral moment of order 8 from edge adjacency mat.
1395	SM09_EA	spectral moment of order 9 from edge adjacency mat.
1396	SM10_EA	spectral moment of order 10 from edge adjacency mat.
1397	SM11_EA	spectral moment of order 11 from edge adjacency mat.
1398	SM12_EA	spectral moment of order 12 from edge adjacency mat.
1399	SM13_EA	spectral moment of order 13 from edge adjacency mat.
1400	SM14_EA	spectral moment of order 14 from edge adjacency mat.
1401	SM15_EA	spectral moment of order 15 from edge adjacency mat.
1402	SM02_EA(ed)	spectral moment of order 2 from edge adjacency mat. weighted by edge degree
1403	SM03_EA(ed)	spectral moment of order 3 from edge adjacency mat. weighted by edge degree
1404	SM04_EA(ed)	spectral moment of order 4 from edge adjacency mat. weighted by edge degree
1405	SM05_EA(ed)	spectral moment of order 5 from edge adjacency mat. weighted by edge degree
1406	SM06_EA(ed)	spectral moment of order 6 from edge adjacency mat. weighted by edge degree
1407	SM07_EA(ed)	spectral moment of order 7 from edge adjacency mat. weighted by edge degree
1408	SM08_EA(ed)	spectral moment of order 8 from edge adjacency mat. weighted by edge degree
1409	SM09_EA(ed)	spectral moment of order 9 from edge adjacency mat. weighted by edge degree
1410	SM10_EA(ed)	spectral moment of order 10 from edge adjacency mat. weighted by edge degree
1411	SM11_EA(ed)	spectral moment of order 11 from edge adjacency mat. weighted by edge degree
1412	SM12_EA(ed)	spectral moment of order 12 from edge adjacency mat. weighted by edge degree
1413	SM13_EA(ed)	spectral moment of order 13 from edge adjacency mat. weighted by edge degree
1414	SM14_EA(ed)	spectral moment of order 14 from edge adjacency mat. weighted by edge degree
1415	SM15_EA(ed)	spectral moment of order 15 from edge adjacency mat. weighted by edge degree
1416	SM02_EA(bo)	spectral moment of order 2 from edge adjacency mat. weighted by bond order
1417	SM03_EA(bo)	spectral moment of order 3 from edge adjacency mat. weighted by bond order
1418	SM04_EA(bo)	spectral moment of order 4 from edge adjacency mat. weighted by bond order
1419	SM05_EA(bo)	spectral moment of order 5 from edge adjacency mat. weighted by bond order
1420	SM06_EA(bo)	spectral moment of order 6 from edge adjacency mat. weighted by bond order
1421	SM07_EA(bo)	spectral moment of order 7 from edge adjacency mat. weighted by bond order
1422	SM08_EA(bo)	spectral moment of order 8 from edge adjacency mat. weighted by bond order
1423	SM09_EA(bo)	spectral moment of order 9 from edge adjacency mat. weighted by bond order
1424	SM10_EA(bo)	spectral moment of order 10 from edge adjacency mat. weighted by bond order
1425	SM11_EA(bo)	spectral moment of order 11 from edge adjacency mat. weighted by bond order
1426	SM12_EA(bo)	spectral moment of order 12 from edge adjacency mat. weighted by bond order
1427	SM13_EA(bo)	spectral moment of order 13 from edge adjacency mat. weighted by bond order
1428	SM14_EA(bo)	spectral moment of order 14 from edge adjacency mat. weighted by bond order
1429	SM15_EA(bo)	spectral moment of order 15 from edge adjacency mat. weighted by bond order
1430	SM02_EA(dm)	spectral moment of order 2 from edge adjacency mat. weighted by dipole moment
1431	SM03_EA(dm)	spectral moment of order 3 from edge adjacency mat. weighted by dipole moment
1432	SM04_EA(dm)	spectral moment of order 4 from edge adjacency mat. weighted by dipole moment
1433	SM05_EA(dm)	spectral moment of order 5 from edge adjacency mat. weighted by dipole moment
1434	SM06_EA(dm)	spectral moment of order 6 from edge adjacency mat. weighted by dipole moment

1435	SM07_EA(dm)	spectral moment of order 7 from edge adjacency mat. weighted by dipole moment
1436	SM08_EA(dm)	spectral moment of order 8 from edge adjacency mat. weighted by dipole moment
1437	SM09_EA(dm)	spectral moment of order 9 from edge adjacency mat. weighted by dipole moment
1438	SM10_EA(dm)	spectral moment of order 10 from edge adjacency mat. weighted by dipole moment
1439	SM11_EA(dm)	spectral moment of order 11 from edge adjacency mat. weighted by dipole moment
1440	SM12_EA(dm)	spectral moment of order 12 from edge adjacency mat. weighted by dipole moment
1441	SM13_EA(dm)	spectral moment of order 13 from edge adjacency mat. weighted by dipole moment
1442	SM14_EA(dm)	spectral moment of order 14 from edge adjacency mat. weighted by dipole moment
1443	SM15_EA(dm)	spectral moment of order 15 from edge adjacency mat. weighted by dipole moment
1444	SM02_EA(ri)	spectral moment of order 2 from edge adjacency mat. weighted by resonance integral
1445	SM03_EA(ri)	spectral moment of order 3 from edge adjacency mat. weighted by resonance integral
1446	SM04_EA(ri)	spectral moment of order 4 from edge adjacency mat. weighted by resonance integral
1447	SM05_EA(ri)	spectral moment of order 5 from edge adjacency mat. weighted by resonance integral
1448	SM06_EA(ri)	spectral moment of order 6 from edge adjacency mat. weighted by resonance integral
1449	SM07_EA(ri)	spectral moment of order 7 from edge adjacency mat. weighted by resonance integral
1450	SM08_EA(ri)	spectral moment of order 8 from edge adjacency mat. weighted by resonance integral
1451	SM09_EA(ri)	spectral moment of order 9 from edge adjacency mat. weighted by resonance integral
1452	SM10_EA(ri)	spectral moment of order 10 from edge adjacency mat. weighted by resonance integral
1453	SM11_EA(ri)	spectral moment of order 11 from edge adjacency mat. weighted by resonance integral
1454	SM12_EA(ri)	spectral moment of order 12 from edge adjacency mat. weighted by resonance integral
1455	SM13_EA(ri)	spectral moment of order 13 from edge adjacency mat. weighted by resonance integral
1456	SM14_EA(ri)	spectral moment of order 14 from edge adjacency mat. weighted by resonance integral
1457	SM15_EA(ri)	spectral moment of order 15 from edge adjacency mat. weighted by resonance integral
1458	SM02_AEA(ed)	spectral moment of order 2 from augmented edge adjacency mat. weighted by edge degree
1459	SM03_AEA(ed)	spectral moment of order 3 from augmented edge adjacency mat. weighted by edge degree
1460	SM04_AEA(ed)	spectral moment of order 4 from augmented edge adjacency mat. weighted by edge degree
1461	SM05_AEA(ed)	spectral moment of order 5 from augmented edge adjacency mat. weighted by edge degree
1462	SM06_AEA(ed)	spectral moment of order 6 from augmented edge adjacency mat. weighted by edge degree
1463	SM07_AEA(ed)	spectral moment of order 7 from augmented edge adjacency mat. weighted by edge degree
1464	SM08_AEA(ed)	spectral moment of order 8 from augmented edge adjacency mat. weighted by edge degree
1465	SM09_AEA(ed)	spectral moment of order 9 from augmented edge adjacency mat. weighted by edge degree
1466	SM10_AEA(ed)	spectral moment of order 10 from augmented edge adjacency mat. weighted by edge degree
1467	SM11_AEA(ed)	spectral moment of order 11 from augmented edge adjacency mat. weighted by edge degree
1468	SM12_AEA(ed)	spectral moment of order 12 from augmented edge adjacency mat. weighted by edge degree
1469	SM13_AEA(ed)	spectral moment of order 13 from augmented edge adjacency mat. weighted by edge degree
1470	SM14_AEA(ed)	spectral moment of order 14 from augmented edge adjacency mat. weighted by edge degree
1471	SM15_AEA(ed)	spectral moment of order 15 from augmented edge adjacency mat. weighted by edge degree
1472	SM02_AEA(bo)	spectral moment of order 2 from augmented edge adjacency mat. weighted by bond order
1473	SM03_AEA(bo)	spectral moment of order 3 from augmented edge adjacency mat. weighted by bond order
1474	SM04_AEA(bo)	spectral moment of order 4 from augmented edge adjacency mat. weighted by bond order
1475	SM05_AEA(bo)	spectral moment of order 5 from augmented edge adjacency mat. weighted by bond order
1476	SM06_AEA(bo)	spectral moment of order 6 from augmented edge adjacency mat. weighted by bond order

1477	SM07_AEA(bo)	spectral moment of order 7 from augmented edge adjacency mat. weighted by bond order
1478	SM08_AEA(bo)	spectral moment of order 8 from augmented edge adjacency mat. weighted by bond order
1479	SM09_AEA(bo)	spectral moment of order 9 from augmented edge adjacency mat. weighted by bond order
1480	SM10_AEA(bo)	spectral moment of order 10 from augmented edge adjacency mat. weighted by bond order
1481	SM11_AEA(bo)	spectral moment of order 11 from augmented edge adjacency mat. weighted by bond order
1482	SM12_AEA(bo)	spectral moment of order 12 from augmented edge adjacency mat. weighted by bond order
1483	SM13_AEA(bo)	spectral moment of order 13 from augmented edge adjacency mat. weighted by bond order
1484	SM14_AEA(bo)	spectral moment of order 14 from augmented edge adjacency mat. weighted by bond order
1485	SM15_AEA(bo)	spectral moment of order 15 from augmented edge adjacency mat. weighted by bond order
1486	SM02_AEA(dm)	spectral moment of order 2 from augmented edge adjacency mat. weighted by dipole moment
1487	SM03_AEA(dm)	spectral moment of order 3 from augmented edge adjacency mat. weighted by dipole moment
1488	SM04_AEA(dm)	spectral moment of order 4 from augmented edge adjacency mat. weighted by dipole moment
1489	SM05_AEA(dm)	spectral moment of order 5 from augmented edge adjacency mat. weighted by dipole moment
1490	SM06_AEA(dm)	spectral moment of order 6 from augmented edge adjacency mat. weighted by dipole moment
1491	SM07_AEA(dm)	spectral moment of order 7 from augmented edge adjacency mat. weighted by dipole moment
1492	SM08_AEA(dm)	spectral moment of order 8 from augmented edge adjacency mat. weighted by dipole moment
1493	SM09_AEA(dm)	spectral moment of order 9 from augmented edge adjacency mat. weighted by dipole moment
1494	SM10_AEA(dm)	spectral moment of order 10 from augmented edge adjacency mat. weighted by dipole moment
1495	SM11_AEA(dm)	spectral moment of order 11 from augmented edge adjacency mat. weighted by dipole moment
1496	SM12_AEA(dm)	spectral moment of order 12 from augmented edge adjacency mat. weighted by dipole moment
1497	SM13_AEA(dm)	spectral moment of order 13 from augmented edge adjacency mat. weighted by dipole moment
1498	SM14_AEA(dm)	spectral moment of order 14 from augmented edge adjacency mat. weighted by dipole moment
1499	SM15_AEA(dm)	spectral moment of order 15 from augmented edge adjacency mat. weighted by dipole moment
1500	SM02_AEA(ri)	spectral moment of order 2 from augmented edge adjacency mat. weighted by resonance integral
1501	SM03_AEA(ri)	spectral moment of order 3 from augmented edge adjacency mat. weighted by resonance integral
1502	SM04_AEA(ri)	spectral moment of order 4 from augmented edge adjacency mat. weighted by resonance integral
1503	SM05_AEA(ri)	spectral moment of order 5 from augmented edge adjacency mat. weighted by resonance integral
1504	SM06_AEA(ri)	spectral moment of order 6 from augmented edge adjacency mat. weighted by resonance integral
1505	SM07_AEA(ri)	spectral moment of order 7 from augmented edge adjacency mat. weighted by resonance integral
1506	SM08_AEA(ri)	spectral moment of order 8 from augmented edge adjacency mat. weighted by resonance integral
1507	SM09_AEA(ri)	spectral moment of order 9 from augmented edge adjacency mat. weighted by resonance integral
1508	SM10_AEA(ri)	spectral moment of order 10 from augmented edge adjacency mat. weighted by resonance integral
1509	SM11_AEA(ri)	spectral moment of order 11 from augmented edge adjacency mat. weighted by resonance integral
1510	SM12_AEA(ri)	spectral moment of order 12 from augmented edge adjacency mat. weighted by resonance integral
1511	SM13_AEA(ri)	spectral moment of order 13 from augmented edge adjacency mat. weighted by resonance integral
1512	SM14_AEA(ri)	spectral moment of order 14 from augmented edge adjacency mat. weighted by resonance integral
1513	SM15_AEA(ri)	spectral moment of order 15 from augmented edge adjacency mat. weighted by resonance integral
1514	Eig01_EA	eigenvalue n. 1 from edge adjacency mat.
1515	Eig02_EA	eigenvalue n. 2 from edge adjacency mat.
1516	Eig03_EA	eigenvalue n. 3 from edge adjacency mat.
1517	Eig04_EA	eigenvalue n. 4 from edge adjacency mat.
1518	Eig05_EA	eigenvalue n. 5 from edge adjacency mat.

1519	Eig06_EA	eigenvalue n. 6 from edge adjacency mat.
1520	Eig07_EA	eigenvalue n. 7 from edge adjacency mat.
1521	Eig08_EA	eigenvalue n. 8 from edge adjacency mat.
1522	Eig09_EA	eigenvalue n. 9 from edge adjacency mat.
1523	Eig10_EA	eigenvalue n. 10 from edge adjacency mat.
1524	Eig11_EA	eigenvalue n. 11 from edge adjacency mat.
1525	Eig12_EA	eigenvalue n. 12 from edge adjacency mat.
1526	Eig13_EA	eigenvalue n. 13 from edge adjacency mat.
1527	Eig14_EA	eigenvalue n. 14 from edge adjacency mat.
1528	Eig15_EA	eigenvalue n. 15 from edge adjacency mat.
1529	Eig01_EA(ed)	eigenvalue n. 1 from edge adjacency mat. weighted by edge degree
1530	Eig02_EA(ed)	eigenvalue n. 2 from edge adjacency mat. weighted by edge degree
1531	Eig03_EA(ed)	eigenvalue n. 3 from edge adjacency mat. weighted by edge degree
1532	Eig04_EA(ed)	eigenvalue n. 4 from edge adjacency mat. weighted by edge degree
1533	Eig05_EA(ed)	eigenvalue n. 5 from edge adjacency mat. weighted by edge degree
1534	Eig06_EA(ed)	eigenvalue n. 6 from edge adjacency mat. weighted by edge degree
1535	Eig07_EA(ed)	eigenvalue n. 7 from edge adjacency mat. weighted by edge degree
1536	Eig08_EA(ed)	eigenvalue n. 8 from edge adjacency mat. weighted by edge degree
1537	Eig09_EA(ed)	eigenvalue n. 9 from edge adjacency mat. weighted by edge degree
1538	Eig10_EA(ed)	eigenvalue n. 10 from edge adjacency mat. weighted by edge degree
1539	Eig11_EA(ed)	eigenvalue n. 11 from edge adjacency mat. weighted by edge degree
1540	Eig12_EA(ed)	eigenvalue n. 12 from edge adjacency mat. weighted by edge degree
1541	Eig13_EA(ed)	eigenvalue n. 13 from edge adjacency mat. weighted by edge degree
1542	Eig14_EA(ed)	eigenvalue n. 14 from edge adjacency mat. weighted by edge degree
1543	Eig15_EA(ed)	eigenvalue n. 15 from edge adjacency mat. weighted by edge degree
1544	Eig01_EA(bo)	eigenvalue n. 1 from edge adjacency mat. weighted by bond order
1545	Eig02_EA(bo)	eigenvalue n. 2 from edge adjacency mat. weighted by bond order
1546	Eig03_EA(bo)	eigenvalue n. 3 from edge adjacency mat. weighted by bond order
1547	Eig04_EA(bo)	eigenvalue n. 4 from edge adjacency mat. weighted by bond order
1548	Eig05_EA(bo)	eigenvalue n. 5 from edge adjacency mat. weighted by bond order
1549	Eig06_EA(bo)	eigenvalue n. 6 from edge adjacency mat. weighted by bond order
1550	Eig07_EA(bo)	eigenvalue n. 7 from edge adjacency mat. weighted by bond order
1551	Eig08_EA(bo)	eigenvalue n. 8 from edge adjacency mat. weighted by bond order
1552	Eig09_EA(bo)	eigenvalue n. 9 from edge adjacency mat. weighted by bond order
1553	Eig10_EA(bo)	eigenvalue n. 10 from edge adjacency mat. weighted by bond order
1554	Eig11_EA(bo)	eigenvalue n. 11 from edge adjacency mat. weighted by bond order
1555	Eig12_EA(bo)	eigenvalue n. 12 from edge adjacency mat. weighted by bond order
1556	Eig13_EA(bo)	eigenvalue n. 13 from edge adjacency mat. weighted by bond order
1557	Eig14_EA(bo)	eigenvalue n. 14 from edge adjacency mat. weighted by bond order
1558	Eig15_EA(bo)	eigenvalue n. 15 from edge adjacency mat. weighted by bond order
1559	Eig01_EA(dm)	eigenvalue n. 1 from edge adjacency mat. weighted by dipole moment
1560	Eig02_EA(dm)	eigenvalue n. 2 from edge adjacency mat. weighted by dipole moment

1561	Eig03_EA(dm)	eigenvalue n. 3 from edge adjacency mat. weighted by dipole moment
1562	Eig04_EA(dm)	eigenvalue n. 4 from edge adjacency mat. weighted by dipole moment
1563	Eig05_EA(dm)	eigenvalue n. 5 from edge adjacency mat. weighted by dipole moment
1564	Eig06_EA(dm)	eigenvalue n. 6 from edge adjacency mat. weighted by dipole moment
1565	Eig07_EA(dm)	eigenvalue n. 7 from edge adjacency mat. weighted by dipole moment
1566	Eig08_EA(dm)	eigenvalue n. 8 from edge adjacency mat. weighted by dipole moment
1567	Eig09_EA(dm)	eigenvalue n. 9 from edge adjacency mat. weighted by dipole moment
1568	Eig10_EA(dm)	eigenvalue n. 10 from edge adjacency mat. weighted by dipole moment
1569	Eig11_EA(dm)	eigenvalue n. 11 from edge adjacency mat. weighted by dipole moment
1570	Eig12_EA(dm)	eigenvalue n. 12 from edge adjacency mat. weighted by dipole moment
1571	Eig13_EA(dm)	eigenvalue n. 13 from edge adjacency mat. weighted by dipole moment
1572	Eig14_EA(dm)	eigenvalue n. 14 from edge adjacency mat. weighted by dipole moment
1573	Eig15_EA(dm)	eigenvalue n. 15 from edge adjacency mat. weighted by dipole moment
1574	Eig01_EA(ri)	eigenvalue n. 1 from edge adjacency mat. weighted by resonance integral
1575	Eig02_EA(ri)	eigenvalue n. 2 from edge adjacency mat. weighted by resonance integral
1576	Eig03_EA(ri)	eigenvalue n. 3 from edge adjacency mat. weighted by resonance integral
1577	Eig04_EA(ri)	eigenvalue n. 4 from edge adjacency mat. weighted by resonance integral
1578	Eig05_EA(ri)	eigenvalue n. 5 from edge adjacency mat. weighted by resonance integral
1579	Eig06_EA(ri)	eigenvalue n. 6 from edge adjacency mat. weighted by resonance integral
1580	Eig07_EA(ri)	eigenvalue n. 7 from edge adjacency mat. weighted by resonance integral
1581	Eig08_EA(ri)	eigenvalue n. 8 from edge adjacency mat. weighted by resonance integral
1582	Eig09_EA(ri)	eigenvalue n. 9 from edge adjacency mat. weighted by resonance integral
1583	Eig10_EA(ri)	eigenvalue n. 10 from edge adjacency mat. weighted by resonance integral
1584	Eig11_EA(ri)	eigenvalue n. 11 from edge adjacency mat. weighted by resonance integral
1585	Eig12_EA(ri)	eigenvalue n. 12 from edge adjacency mat. weighted by resonance integral
1586	Eig13_EA(ri)	eigenvalue n. 13 from edge adjacency mat. weighted by resonance integral
1587	Eig14_EA(ri)	eigenvalue n. 14 from edge adjacency mat. weighted by resonance integral
1588	Eig15_EA(ri)	eigenvalue n. 15 from edge adjacency mat. weighted by resonance integral
1589	Eig01_AEA(ed)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by edge degree
1590	Eig02_AEA(ed)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by edge degree
1591	Eig03_AEA(ed)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by edge degree
1592	Eig04_AEA(ed)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by edge degree
1593	Eig05_AEA(ed)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by edge degree
1594	Eig06_AEA(ed)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by edge degree
1595	Eig07_AEA(ed)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by edge degree
1596	Eig08_AEA(ed)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by edge degree
1597	Eig09_AEA(ed)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by edge degree
1598	Eig10_AEA(ed)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by edge degree
1599	Eig11_AEA(ed)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by edge degree
1600	Eig12_AEA(ed)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by edge degree
1601	Eig13_AEA(ed)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by edge degree
1602	Eig14_AEA(ed)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by edge degree

1603	Eig15_AEA(ed)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by edge degree
1604	Eig01_AEA(bo)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by bond order
1605	Eig02_AEA(bo)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by bond order
1606	Eig03_AEA(bo)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by bond order
1607	Eig04_AEA(bo)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by bond order
1608	Eig05_AEA(bo)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by bond order
1609	Eig06_AEA(bo)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by bond order
1610	Eig07_AEA(bo)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by bond order
1611	Eig08_AEA(bo)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by bond order
1612	Eig09_AEA(bo)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by bond order
1613	Eig10_AEA(bo)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by bond order
1614	Eig11_AEA(bo)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by bond order
1615	Eig12_AEA(bo)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by bond order
1616	Eig13_AEA(bo)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by bond order
1617	Eig14_AEA(bo)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by bond order
1618	Eig15_AEA(bo)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by bond order
1619	Eig01_AEA(dm)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment
1620	Eig02_AEA(dm)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by dipole moment
1621	Eig03_AEA(dm)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by dipole moment
1622	Eig04_AEA(dm)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by dipole moment
1623	Eig05_AEA(dm)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by dipole moment
1624	Eig06_AEA(dm)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by dipole moment
1625	Eig07_AEA(dm)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by dipole moment
1626	Eig08_AEA(dm)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by dipole moment
1627	Eig09_AEA(dm)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by dipole moment
1628	Eig10_AEA(dm)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by dipole moment
1629	Eig11_AEA(dm)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by dipole moment
1630	Eig12_AEA(dm)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by dipole moment
1631	Eig13_AEA(dm)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by dipole moment
1632	Eig14_AEA(dm)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by dipole moment
1633	Eig15_AEA(dm)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by dipole moment
1634	Eig01_AEA(ri)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by resonance integral
1635	Eig02_AEA(ri)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by resonance integral
1636	Eig03_AEA(ri)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by resonance integral
1637	Eig04_AEA(ri)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by resonance integral
1638	Eig05_AEA(ri)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by resonance integral
1639	Eig06_AEA(ri)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by resonance integral
1640	Eig07_AEA(ri)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by resonance integral
1641	Eig08_AEA(ri)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by resonance integral
1642	Eig09_AEA(ri)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by resonance integral
1643	Eig10_AEA(ri)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by resonance integral
1644	Eig11_AEA(ri)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by resonance integral

1645	Eig12_AEA(ri)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by resonance integral
1646	Eig13_AEA(ri)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by resonance integral
1647	Eig14_AEA(ri)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by resonance integral
1648	Eig15_AEA(ri)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by resonance integral

13. Geometrical descriptors

No.	Name	Description
1649	G1	gravitational index G1
1650	G2	gravitational index G2 (bond-restricted)
1651	RGyr	radius of gyration (mass weighted)
1652	SPAN	span R
1653	SPAM	average span R
1654	MEcc	molecular eccentricity
1655	SPH	spherosity
1656	ASP	asphericity
1657	PJI3	3D Petitjean shape index
1658	L/Bw	length-to-breadth ratio by WHIM
1659	HOMA	Harmonic Oscillator Model of Aromaticity index
1660	CMBL	conjugated maximum bond length
1661	AROM	aromaticity index
1662	HOMT	HOMA total
1663	DISPm	displacement value / weighted by mass
1664	QXXm	quadrupole x-component value / weighted by mass
1665	QYYm	quadrupole y-component value / weighted by mass
1666	QZZm	quadrupole z-component value / weighted by mass
1667	DISPv	displacement value / weighted by van der Waals volume
1668	QXXv	quadrupole x-component value / weighted by van der Waals volume
1669	QYYv	quadrupole y-component value / weighted by van der Waals volume
1670	QZZv	quadrupole z-component value / weighted by van der Waals volume
1671	DISPe	displacement value / weighted by Sanderson electronegativity
1672	QXXe	quadrupole x-component value / weighted by Sanderson electronegativity
1673	QYYe	quadrupole y-component value / weighted by Sanderson electronegativity
1674	QZZe	quadrupole z-component value / weighted by Sanderson electronegativity
1675	DISPp	displacement value / weighted by polarizability
1676	QXXp	quadrupole x-component value / weighted by polarizability
1677	QYYp	quadrupole y-component value / weighted by polarizability
1678	QZZp	quadrupole z-component value / weighted by polarizability
1679	DISPi	displacement value / weighted by ionization potential
1680	QXXi	quadrupole x-component value / weighted by ionization potential
1681	QYYi	quadrupole y-component value / weighted by ionization potential
1682	QZZi	quadrupole z-component value / weighted by ionization potential
1683	DISPs	displacement value / weighted by I-state

1684	QXXs	quadrupole x-component value / weighted by I-state
1685	QYYs	quadrupole y-component value / weighted by I-state
1686	QZZs	quadrupole z-component value / weighted by I-state

14. 3D matrix-based descriptors

No.	Name	Description
1687	Wi_G	Wiener-like index from geometrical matrix
1688	WiA_G	average Wiener-like index from geometrical matrix
1689	AVS_G	average vertex sum from geometrical matrix
1690	H_G	Harary-like index from geometrical matrix
1691	Chi_G	Randic-like index from geometrical matrix
1692	ChiA_G	average Randic-like index from geometrical matrix
1693	J_G	Balaban-like index from geometrical matrix
1694	HyWi_G	hyper-Wiener-like index from geometrical matrix
1695	SpAbs_G	graph energy from geometrical matrix
1696	SpPos_G	spectral positive sum from geometrical matrix
1697	SpPosA_G	normalized spectral positive sum from geometrical matrix
1698	SpPosLog_G	logarithmic spectral positive sum from geometrical matrix
1699	SpMax_G	leading eigenvalue from geometrical matrix
1700	SpMaxA_G	normalized leading eigenvalue from geometrical matrix
1701	SpDiam_G	spectral diameter from geometrical matrix
1702	SpAD_G	spectral absolute deviation from geometrical matrix
1703	SpMAD_G	spectral mean absolute deviation from geometrical matrix
1704	Ho_G	Hosoya-like index (log function) from geometrical matrix
1705	EE_G	Estrada-like index (log function) from geometrical matrix
1706	SM2_G	spectral moment of order 2 from geometrical matrix
1707	SM3_G	spectral moment of order 3 from geometrical matrix
1708	SM4_G	spectral moment of order 4 from geometrical matrix
1709	SM5_G	spectral moment of order 5 from geometrical matrix
1710	SM6_G	spectral moment of order 6 from geometrical matrix
1711	VE1_G	coefficient sum of the last eigenvector (absolute values) from geometrical matrix
1712	VE2_G	average coefficient of the last eigenvector (absolute values) from geometrical matrix
1713	VE3_G	logarithmic coefficient sum of the last eigenvector (absolute values) from geometrical matrix
1714	VE1sign_G	coefficient sum of the last eigenvector from geometrical matrix
1715	VE2sign_G	average coefficient of the last eigenvector from geometrical matrix
1716	VE3sign_G	logarithmic coefficient sum of the last eigenvector from geometrical matrix
1717	VR1_G	Randic-like eigenvector-based index from geometrical matrix
1718	VR2_G	normalized Randic-like eigenvector-based index from geometrical matrix
1719	VR3_G	logarithmic Randic-like eigenvector-based index from geometrical matrix
1720	Wi_RG	Wiener-like index from reciprocal squared geometrical matrix
1721	WiA_RG	average Wiener-like index from reciprocal squared geometrical matrix
1722	AVS_RG	average vertex sum from reciprocal squared geometrical matrix

1723	H_RG	Harary-like index from reciprocal squared geometrical matrix
1724	Chi_RG	Randic-like index from reciprocal squared geometrical matrix
1725	ChiA_RG	average Randic-like index from reciprocal squared geometrical matrix
1726	J_RG	Balaban-like index from reciprocal squared geometrical matrix
1727	HyWi_RG	hyper-Wiener-like index from reciprocal squared geometrical matrix
1728	SpAbs_RG	graph energy from reciprocal squared geometrical matrix
1729	SpPos_RG	spectral positive sum from reciprocal squared geometrical matrix
1730	SpPosA_RG	normalized spectral positive sum from reciprocal squared geometrical matrix
1731	SpPosLog_RG	logarithmic spectral positive sum from reciprocal squared geometrical matrix
1732	SpMax_RG	leading eigenvalue from reciprocal squared geometrical matrix
1733	SpMaxA_RG	normalized leading eigenvalue from reciprocal squared geometrical matrix
1734	SpDiam_RG	spectral diameter from reciprocal squared geometrical matrix
1735	SpAD_RG	spectral absolute deviation from reciprocal squared geometrical matrix
1736	SpMAD_RG	spectral mean absolute deviation from reciprocal squared geometrical matrix
1737	Ho_RG	Hosoya-like index (log function) from reciprocal squared geometrical matrix
1738	EE_RG	Estrada-like index (log function) from reciprocal squared geometrical matrix
1739	SM2_RG	spectral moment of order 2 from reciprocal squared geometrical matrix
1740	SM3_RG	spectral moment of order 3 from reciprocal squared geometrical matrix
1741	SM4_RG	spectral moment of order 4 from reciprocal squared geometrical matrix
1742	SM5_RG	spectral moment of order 5 from reciprocal squared geometrical matrix
1743	SM6_RG	spectral moment of order 6 from reciprocal squared geometrical matrix
1744	VE1_RG	coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix
1745	VE2_RG	average coefficient of the last eigenvector (absolute values) from reciprocal squared geometrical matrix
1746	VE3_RG	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix
1747	VE1sign_RG	coefficient sum of the last eigenvector from reciprocal squared geometrical matrix
1748	VE2sign_RG	average coefficient of the last eigenvector from reciprocal squared geometrical matrix
1749	VE3sign_RG	logarithmic coefficient sum of the last eigenvector from reciprocal squared geometrical matrix
1750	VR1_RG	Randic-like eigenvector-based index from reciprocal squared geometrical matrix
1751	VR2_RG	normalized Randic-like eigenvector-based index from reciprocal squared geometrical matrix
1752	VR3_RG	logarithmic Randic-like eigenvector-based index from reciprocal squared geometrical matrix
1753	Wi_G/D	Wiener-like index from distance/distance matrix
1754	WiA_G/D	average Wiener-like index from distance/distance matrix
1755	AVS_G/D	average vertex sum from distance/distance matrix
1756	H_G/D	Harary-like index from distance/distance matrix
1757	Chi_G/D	Randic-like index from distance/distance matrix
1758	ChiA_G/D	average Randic-like index from distance/distance matrix
1759	J_G/D	Balaban-like index from distance/distance matrix
1760	HyWi_G/D	hyper-Wiener-like index from distance/distance matrix
1761	SpAbs_G/D	graph energy from distance/distance matrix
1762	SpPos_G/D	spectral positive sum from distance/distance matrix
1763	SpPosA_G/D	normalized spectral positive sum from distance/distance matrix
1764	SpPosLog_G/D	logarithmic spectral positive sum from distance/distance matrix

1765	SpMax_G/D	leading eigenvalue from distance/distance matrix
1766	SpMaxA_G/D	normalized leading eigenvalue from distance/distance matrix (folding degree index)
1767	SpDiam_G/D	spectral diameter from distance/distance matrix
1768	SpAD_G/D	spectral absolute deviation from distance/distance matrix
1769	SpMAD_G/D	spectral mean absolute deviation from distance/distance matrix
1770	Ho_G/D	Hosoya-like index (log function) from distance/distance matrix
1771	EE_G/D	Estrada-like index (log function) from distance/distance matrix
1772	SM2_G/D	spectral moment of order 2 from distance/distance matrix
1773	SM3_G/D	spectral moment of order 3 from distance/distance matrix
1774	SM4_G/D	spectral moment of order 4 from distance/distance matrix
1775	SM5_G/D	spectral moment of order 5 from distance/distance matrix
1776	SM6_G/D	spectral moment of order 6 from distance/distance matrix
1777	VE1_G/D	coefficient sum of the last eigenvector (absolute values) from distance/distance matrix
1778	VE2_G/D	average coefficient of the last eigenvector (absolute values) from distance/distance matrix
1779	VE3_G/D	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/distance matrix
1780	VE1sign_G/D	coefficient sum of the last eigenvector from distance/distance matrix
1781	VE2sign_G/D	average coefficient of the last eigenvector from distance/distance matrix
1782	VE3sign_G/D	logarithmic coefficient sum of the last eigenvector from distance/distance matrix
1783	VR1_G/D	Randic-like eigenvector-based index from distance/distance matrix
1784	VR2_G/D	normalized Randic-like eigenvector-based index from distance/distance matrix
1785	VR3_G/D	logarithmic Randic-like eigenvector-based index from distance/distance matrix
1786	Wi_Coulomb	Wiener-like index from Coulomb matrix
1787	WiA_Coulomb	average Wiener-like index from Coulomb matrix
1788	AVS_Coulomb	average vertex sum from Coulomb matrix
1789	H_Coulomb	Harary-like index from Coulomb matrix
1790	Chi_Coulomb	Randic-like index from Coulomb matrix
1791	ChiA_Coulomb	average Randic-like index from Coulomb matrix
1792	J_Coulomb	Balaban-like index from Coulomb matrix
1793	HyWi_Coulomb	hyper-Wiener-like index from Coulomb matrix
1794	SpAbs_Coulomb	graph energy from Coulomb matrix
1795	SpPos_Coulomb	spectral positive sum from Coulomb matrix
1796	SpPosA_Coulomb	normalized spectral positive sum from Coulomb matrix
1797	SpPosLog_Coulomb	logarithmic spectral positive sum from Coulomb matrix
1798	SpMax_Coulomb	leading eigenvalue from Coulomb matrix
1799	SpMaxA_Coulomb	normalized leading eigenvalue from Coulomb matrix
1800	SpDiam_Coulomb	spectral diameter from Coulomb matrix
1801	SpAD_Coulomb	spectral absolute deviation from Coulomb matrix
1802	SpMAD_Coulomb	spectral mean absolute deviation from Coulomb matrix
1803	Ho_Coulomb	Hosoya-like index (log function) from Coulomb matrix
1804	EE_Coulomb	Estrada-like index (log function) from Coulomb matrix
1805	SM2_Coulomb	spectral moment of order 2 from Coulomb matrix
1806	SM3_Coulomb	spectral moment of order 3 from Coulomb matrix

1807	SM4_Coulomb	spectral moment of order 4 from Coulomb matrix
1808	SM5_Coulomb	spectral moment of order 5 from Coulomb matrix
1809	SM6_Coulomb	spectral moment of order 6 from Coulomb matrix
1810	VE1_Coulomb	coefficient sum of the last eigenvector (absolute values) from Coulomb matrix
1811	VE2_Coulomb	average coefficient of the last eigenvector (absolute values) from Coulomb matrix
1812	VE3_Coulomb	logarithmic coefficient sum of the last eigenvector (absolute values) from Coulomb matrix
1813	VE1sign_Coulomb	coefficient sum of the last eigenvector from Coulomb matrix
1814	VE2sign_Coulomb	average coefficient of the last eigenvector from Coulomb matrix
1815	VE3sign_Coulomb	logarithmic coefficient sum of the last eigenvector from Coulomb matrix
1816	VR1_Coulomb	Randic-like eigenvector-based index from Coulomb matrix
1817	VR2_Coulomb	normalized Randic-like eigenvector-based index from Coulomb matrix
1818	VR3_Coulomb	logarithmic Randic-like eigenvector-based index from Coulomb matrix

15. 3D autocorrelations

No.	Name	Description
1819	TDB01u	3D Topological distance based descriptors – lag 1 unweighted
1820	TDB02u	3D Topological distance based descriptors – lag 2 unweighted
1821	TDB03u	3D Topological distance based descriptors – lag 3 unweighted
1822	TDB04u	3D Topological distance based descriptors – lag 4 unweighted
1823	TDB05u	3D Topological distance based descriptors – lag 5 unweighted
1824	TDB06u	3D Topological distance based descriptors – lag 6 unweighted
1825	TDB07u	3D Topological distance based descriptors – lag 7 unweighted
1826	TDB08u	3D Topological distance based descriptors – lag 8 unweighted
1827	TDB09u	3D Topological distance based descriptors – lag 9 unweighted
1828	TDB10u	3D Topological distance based descriptors – lag 10 unweighted
1829	TDB01m	3D Topological distance based descriptors – lag 1 weighted by mass
1830	TDB02m	3D Topological distance based descriptors – lag 2 weighted by mass
1831	TDB03m	3D Topological distance based descriptors – lag 3 weighted by mass
1832	TDB04m	3D Topological distance based descriptors – lag 4 weighted by mass
1833	TDB05m	3D Topological distance based descriptors – lag 5 weighted by mass
1834	TDB06m	3D Topological distance based descriptors – lag 6 weighted by mass
1835	TDB07m	3D Topological distance based descriptors – lag 7 weighted by mass
1836	TDB08m	3D Topological distance based descriptors – lag 8 weighted by mass
1837	TDB09m	3D Topological distance based descriptors – lag 9 weighted by mass
1838	TDB10m	3D Topological distance based descriptors – lag 10 weighted by mass
1839	TDB01v	3D Topological distance based descriptors – lag 1 weighted by van der Waals volume
1840	TDB02v	3D Topological distance based descriptors – lag 2 weighted by van der Waals volume
1841	TDB03v	3D Topological distance based descriptors – lag 3 weighted by van der Waals volume
1842	TDB04v	3D Topological distance based descriptors – lag 4 weighted by van der Waals volume
1843	TDB05v	3D Topological distance based descriptors – lag 5 weighted by van der Waals volume
1844	TDB06v	3D Topological distance based descriptors – lag 6 weighted by van der Waals volume
1845	TDB07v	3D Topological distance based descriptors – lag 7 weighted by van der Waals volume

1846	TDB08v	3D Topological distance based descriptors – lag 8 weighted by van der Waals volume
1847	TDB09v	3D Topological distance based descriptors – lag 9 weighted by van der Waals volume
1848	TDB10v	3D Topological distance based descriptors – lag 10 weighted by van der Waals volume
1849	TDB01e	3D Topological distance based descriptors – lag 1 weighted by Sanderson electronegativity
1850	TDB02e	3D Topological distance based descriptors – lag 2 weighted by Sanderson electronegativity
1851	TDB03e	3D Topological distance based descriptors – lag 3 weighted by Sanderson electronegativity
1852	TDB04e	3D Topological distance based descriptors – lag 4 weighted by Sanderson electronegativity
1853	TDB05e	3D Topological distance based descriptors – lag 5 weighted by Sanderson electronegativity
1854	TDB06e	3D Topological distance based descriptors – lag 6 weighted by Sanderson electronegativity
1855	TDB07e	3D Topological distance based descriptors – lag 7 weighted by Sanderson electronegativity
1856	TDB08e	3D Topological distance based descriptors – lag 8 weighted by Sanderson electronegativity
1857	TDB09e	3D Topological distance based descriptors – lag 9 weighted by Sanderson electronegativity
1858	TDB10e	3D Topological distance based descriptors – lag 10 weighted by Sanderson electronegativity
1859	TDB01p	3D Topological distance based descriptors – lag 1 weighted by polarizability
1860	TDB02p	3D Topological distance based descriptors – lag 2 weighted by polarizability
1861	TDB03p	3D Topological distance based descriptors – lag 3 weighted by polarizability
1862	TDB04p	3D Topological distance based descriptors – lag 4 weighted by polarizability
1863	TDB05p	3D Topological distance based descriptors – lag 5 weighted by polarizability
1864	TDB06p	3D Topological distance based descriptors – lag 6 weighted by polarizability
1865	TDB07p	3D Topological distance based descriptors – lag 7 weighted by polarizability
1866	TDB08p	3D Topological distance based descriptors – lag 8 weighted by polarizability
1867	TDB09p	3D Topological distance based descriptors – lag 9 weighted by polarizability
1868	TDB10p	3D Topological distance based descriptors – lag 10 weighted by polarizability
1869	TDB01i	3D Topological distance based descriptors – lag 1 weighted by ionization potential
1870	TDB02i	3D Topological distance based descriptors – lag 2 weighted by ionization potential
1871	TDB03i	3D Topological distance based descriptors – lag 3 weighted by ionization potential
1872	TDB04i	3D Topological distance based descriptors – lag 4 weighted by ionization potential
1873	TDB05i	3D Topological distance based descriptors – lag 5 weighted by ionization potential
1874	TDB06i	3D Topological distance based descriptors – lag 6 weighted by ionization potential
1875	TDB07i	3D Topological distance based descriptors – lag 7 weighted by ionization potential
1876	TDB08i	3D Topological distance based descriptors – lag 8 weighted by ionization potential
1877	TDB09i	3D Topological distance based descriptors – lag 9 weighted by ionization potential
1878	TDB10i	3D Topological distance based descriptors – lag 10 weighted by ionization potential
1879	TDB01s	3D Topological distance based descriptors – lag 1 weighted by I-state
1880	TDB02s	3D Topological distance based descriptors – lag 2 weighted by I-state
1881	TDB03s	3D Topological distance based descriptors – lag 3 weighted by I-state
1882	TDB04s	3D Topological distance based descriptors – lag 4 weighted by I-state
1883	TDB05s	3D Topological distance based descriptors – lag 5 weighted by I-state
1884	TDB06s	3D Topological distance based descriptors – lag 6 weighted by I-state
1885	TDB07s	3D Topological distance based descriptors – lag 7 weighted by I-state
1886	TDB08s	3D Topological distance based descriptors – lag 8 weighted by I-state
1887	TDB09s	3D Topological distance based descriptors – lag 9 weighted by I-state

1888	TDB10s	3D Topological distance based descriptors – lag 10 weighted by I-state
1889	TDB01r	3D Topological distance based descriptors – lag 1 weighted by covalent radius
1890	TDB02r	3D Topological distance based descriptors – lag 2 weighted by covalent radius
1891	TDB03r	3D Topological distance based descriptors – lag 3 weighted by covalent radius
1892	TDB04r	3D Topological distance based descriptors – lag 4 weighted by covalent radius
1893	TDB05r	3D Topological distance based descriptors – lag 5 weighted by covalent radius
1894	TDB06r	3D Topological distance based descriptors – lag 6 weighted by covalent radius
1895	TDB07r	3D Topological distance based descriptors – lag 7 weighted by covalent radius
1896	TDB08r	3D Topological distance based descriptors – lag 8 weighted by covalent radius
1897	TDB09r	3D Topological distance based descriptors – lag 9 weighted by covalent radius
1898	TDB10r	3D Topological distance based descriptors – lag 10 weighted by covalent radius

16. RDF descriptors

No.	Name	Description
1899	RDF010u	Radial Distribution Function – 010 / unweighted
1900	RDF015u	Radial Distribution Function – 015 / unweighted
1901	RDF020u	Radial Distribution Function – 020 / unweighted
1902	RDF025u	Radial Distribution Function – 025 / unweighted
1903	RDF030u	Radial Distribution Function – 030 / unweighted
1904	RDF035u	Radial Distribution Function – 035 / unweighted
1905	RDF040u	Radial Distribution Function – 040 / unweighted
1906	RDF045u	Radial Distribution Function – 045 / unweighted
1907	RDF050u	Radial Distribution Function – 050 / unweighted
1908	RDF055u	Radial Distribution Function – 055 / unweighted
1909	RDF060u	Radial Distribution Function – 060 / unweighted
1910	RDF065u	Radial Distribution Function – 065 / unweighted
1911	RDF070u	Radial Distribution Function – 070 / unweighted
1912	RDF075u	Radial Distribution Function – 075 / unweighted
1913	RDF080u	Radial Distribution Function – 080 / unweighted
1914	RDF085u	Radial Distribution Function – 085 / unweighted
1915	RDF090u	Radial Distribution Function – 090 / unweighted
1916	RDF095u	Radial Distribution Function – 095 / unweighted
1917	RDF100u	Radial Distribution Function – 100 / unweighted
1918	RDF105u	Radial Distribution Function – 105 / unweighted
1919	RDF110u	Radial Distribution Function – 110 / unweighted
1920	RDF115u	Radial Distribution Function – 115 / unweighted
1921	RDF120u	Radial Distribution Function – 120 / unweighted
1922	RDF125u	Radial Distribution Function – 125 / unweighted
1923	RDF130u	Radial Distribution Function – 130 / unweighted
1924	RDF135u	Radial Distribution Function – 135 / unweighted
1925	RDF140u	Radial Distribution Function – 140 / unweighted
1926	RDF145u	Radial Distribution Function – 145 / unweighted

1927	RDF150u	Radial Distribution Function – 150 / unweighted
1928	RDF155u	Radial Distribution Function – 155 / unweighted
1929	RDF010m	Radial Distribution Function – 010 / weighted by mass
1930	RDF015m	Radial Distribution Function – 015 / weighted by mass
1931	RDF020m	Radial Distribution Function – 020 / weighted by mass
1932	RDF025m	Radial Distribution Function – 025 / weighted by mass
1933	RDF030m	Radial Distribution Function – 030 / weighted by mass
1934	RDF035m	Radial Distribution Function – 035 / weighted by mass
1935	RDF040m	Radial Distribution Function – 040 / weighted by mass
1936	RDF045m	Radial Distribution Function – 045 / weighted by mass
1937	RDF050m	Radial Distribution Function – 050 / weighted by mass
1938	RDF055m	Radial Distribution Function – 055 / weighted by mass
1939	RDF060m	Radial Distribution Function – 060 / weighted by mass
1940	RDF065m	Radial Distribution Function – 065 / weighted by mass
1941	RDF070m	Radial Distribution Function – 070 / weighted by mass
1942	RDF075m	Radial Distribution Function – 075 / weighted by mass
1943	RDF080m	Radial Distribution Function – 080 / weighted by mass
1944	RDF085m	Radial Distribution Function – 085 / weighted by mass
1945	RDF090m	Radial Distribution Function – 090 / weighted by mass
1946	RDF095m	Radial Distribution Function – 095 / weighted by mass
1947	RDF100m	Radial Distribution Function – 100 / weighted by mass
1948	RDF105m	Radial Distribution Function – 105 / weighted by mass
1949	RDF110m	Radial Distribution Function – 110 / weighted by mass
1950	RDF115m	Radial Distribution Function – 115 / weighted by mass
1951	RDF120m	Radial Distribution Function – 120 / weighted by mass
1952	RDF125m	Radial Distribution Function – 125 / weighted by mass
1953	RDF130m	Radial Distribution Function – 130 / weighted by mass
1954	RDF135m	Radial Distribution Function – 135 / weighted by mass
1955	RDF140m	Radial Distribution Function – 140 / weighted by mass
1956	RDF145m	Radial Distribution Function – 145 / weighted by mass
1957	RDF150m	Radial Distribution Function – 150 / weighted by mass
1958	RDF155m	Radial Distribution Function – 155 / weighted by mass
1959	RDF010v	Radial Distribution Function – 010 / weighted by van der Waals volume
1960	RDF015v	Radial Distribution Function – 015 / weighted by van der Waals volume
1961	RDF020v	Radial Distribution Function – 020 / weighted by van der Waals volume
1962	RDF025v	Radial Distribution Function – 025 / weighted by van der Waals volume
1963	RDF030v	Radial Distribution Function – 030 / weighted by van der Waals volume
1964	RDF035v	Radial Distribution Function – 035 / weighted by van der Waals volume
1965	RDF040v	Radial Distribution Function – 040 / weighted by van der Waals volume
1966	RDF045v	Radial Distribution Function – 045 / weighted by van der Waals volume
1967	RDF050v	Radial Distribution Function – 050 / weighted by van der Waals volume
1968	RDF055v	Radial Distribution Function – 055 / weighted by van der Waals volume

1969	RDF060v	Radial Distribution Function – 060 / weighted by van der Waals volume
1970	RDF065v	Radial Distribution Function – 065 / weighted by van der Waals volume
1971	RDF070v	Radial Distribution Function – 070 / weighted by van der Waals volume
1972	RDF075v	Radial Distribution Function – 075 / weighted by van der Waals volume
1973	RDF080v	Radial Distribution Function – 080 / weighted by van der Waals volume
1974	RDF085v	Radial Distribution Function – 085 / weighted by van der Waals volume
1975	RDF090v	Radial Distribution Function – 090 / weighted by van der Waals volume
1976	RDF095v	Radial Distribution Function – 095 / weighted by van der Waals volume
1977	RDF100v	Radial Distribution Function – 100 / weighted by van der Waals volume
1978	RDF105v	Radial Distribution Function – 105 / weighted by van der Waals volume
1979	RDF110v	Radial Distribution Function – 110 / weighted by van der Waals volume
1980	RDF115v	Radial Distribution Function – 115 / weighted by van der Waals volume
1981	RDF120v	Radial Distribution Function – 120 / weighted by van der Waals volume
1982	RDF125v	Radial Distribution Function – 125 / weighted by van der Waals volume
1983	RDF130v	Radial Distribution Function – 130 / weighted by van der Waals volume
1984	RDF135v	Radial Distribution Function – 135 / weighted by van der Waals volume
1985	RDF140v	Radial Distribution Function – 140 / weighted by van der Waals volume
1986	RDF145v	Radial Distribution Function – 145 / weighted by van der Waals volume
1987	RDF150v	Radial Distribution Function – 150 / weighted by van der Waals volume
1988	RDF155v	Radial Distribution Function – 155 / weighted by van der Waals volume
1989	RDF010e	Radial Distribution Function – 010 / weighted by Sanderson electronegativity
1990	RDF015e	Radial Distribution Function – 015 / weighted by Sanderson electronegativity
1991	RDF020e	Radial Distribution Function – 020 / weighted by Sanderson electronegativity
1992	RDF025e	Radial Distribution Function – 025 / weighted by Sanderson electronegativity
1993	RDF030e	Radial Distribution Function – 030 / weighted by Sanderson electronegativity
1994	RDF035e	Radial Distribution Function – 035 / weighted by Sanderson electronegativity
1995	RDF040e	Radial Distribution Function – 040 / weighted by Sanderson electronegativity
1996	RDF045e	Radial Distribution Function – 045 / weighted by Sanderson electronegativity
1997	RDF050e	Radial Distribution Function – 050 / weighted by Sanderson electronegativity
1998	RDF055e	Radial Distribution Function – 055 / weighted by Sanderson electronegativity
1999	RDF060e	Radial Distribution Function – 060 / weighted by Sanderson electronegativity
2000	RDF065e	Radial Distribution Function – 065 / weighted by Sanderson electronegativity
2001	RDF070e	Radial Distribution Function – 070 / weighted by Sanderson electronegativity
2002	RDF075e	Radial Distribution Function – 075 / weighted by Sanderson electronegativity
2003	RDF080e	Radial Distribution Function – 080 / weighted by Sanderson electronegativity
2004	RDF085e	Radial Distribution Function – 085 / weighted by Sanderson electronegativity
2005	RDF090e	Radial Distribution Function – 090 / weighted by Sanderson electronegativity
2006	RDF095e	Radial Distribution Function – 095 / weighted by Sanderson electronegativity
2007	RDF100e	Radial Distribution Function – 100 / weighted by Sanderson electronegativity
2008	RDF105e	Radial Distribution Function – 105 / weighted by Sanderson electronegativity
2009	RDF110e	Radial Distribution Function – 110 / weighted by Sanderson electronegativity
2010	RDF115e	Radial Distribution Function – 115 / weighted by Sanderson electronegativity

2011	RDF120e	Radial Distribution Function – 120 / weighted by Sanderson electronegativity
2012	RDF125e	Radial Distribution Function – 125 / weighted by Sanderson electronegativity
2013	RDF130e	Radial Distribution Function – 130 / weighted by Sanderson electronegativity
2014	RDF135e	Radial Distribution Function – 135 / weighted by Sanderson electronegativity
2015	RDF140e	Radial Distribution Function – 140 / weighted by Sanderson electronegativity
2016	RDF145e	Radial Distribution Function – 145 / weighted by Sanderson electronegativity
2017	RDF150e	Radial Distribution Function – 150 / weighted by Sanderson electronegativity
2018	RDF155e	Radial Distribution Function – 155 / weighted by Sanderson electronegativity
2019	RDF010p	Radial Distribution Function – 010 / weighted by polarizability
2020	RDF015p	Radial Distribution Function – 015 / weighted by polarizability
2021	RDF020p	Radial Distribution Function – 020 / weighted by polarizability
2022	RDF025p	Radial Distribution Function – 025 / weighted by polarizability
2023	RDF030p	Radial Distribution Function – 030 / weighted by polarizability
2024	RDF035p	Radial Distribution Function – 035 / weighted by polarizability
2025	RDF040p	Radial Distribution Function – 040 / weighted by polarizability
2026	RDF045p	Radial Distribution Function – 045 / weighted by polarizability
2027	RDF050p	Radial Distribution Function – 050 / weighted by polarizability
2028	RDF055p	Radial Distribution Function – 055 / weighted by polarizability
2029	RDF060p	Radial Distribution Function – 060 / weighted by polarizability
2030	RDF065p	Radial Distribution Function – 065 / weighted by polarizability
2031	RDF070p	Radial Distribution Function – 070 / weighted by polarizability
2032	RDF075p	Radial Distribution Function – 075 / weighted by polarizability
2033	RDF080p	Radial Distribution Function – 080 / weighted by polarizability
2034	RDF085p	Radial Distribution Function – 085 / weighted by polarizability
2035	RDF090p	Radial Distribution Function – 090 / weighted by polarizability
2036	RDF095p	Radial Distribution Function – 095 / weighted by polarizability
2037	RDF100p	Radial Distribution Function – 100 / weighted by polarizability
2038	RDF105p	Radial Distribution Function – 105 / weighted by polarizability
2039	RDF110p	Radial Distribution Function – 110 / weighted by polarizability
2040	RDF115p	Radial Distribution Function – 115 / weighted by polarizability
2041	RDF120p	Radial Distribution Function – 120 / weighted by polarizability
2042	RDF125p	Radial Distribution Function – 125 / weighted by polarizability
2043	RDF130p	Radial Distribution Function – 130 / weighted by polarizability
2044	RDF135p	Radial Distribution Function – 135 / weighted by polarizability
2045	RDF140p	Radial Distribution Function – 140 / weighted by polarizability
2046	RDF145p	Radial Distribution Function – 145 / weighted by polarizability
2047	RDF150p	Radial Distribution Function – 150 / weighted by polarizability
2048	RDF155p	Radial Distribution Function – 155 / weighted by polarizability
2049	RDF010i	Radial Distribution Function – 010 / weighted by ionization potential
2050	RDF015i	Radial Distribution Function – 015 / weighted by ionization potential
2051	RDF020i	Radial Distribution Function – 020 / weighted by ionization potential
2052	RDF025i	Radial Distribution Function – 025 / weighted by ionization potential

2053	RDF030i	Radial Distribution Function – 030 / weighted by ionization potential
2054	RDF035i	Radial Distribution Function – 035 / weighted by ionization potential
2055	RDF040i	Radial Distribution Function – 040 / weighted by ionization potential
2056	RDF045i	Radial Distribution Function – 045 / weighted by ionization potential
2057	RDF050i	Radial Distribution Function – 050 / weighted by ionization potential
2058	RDF055i	Radial Distribution Function – 055 / weighted by ionization potential
2059	RDF060i	Radial Distribution Function – 060 / weighted by ionization potential
2060	RDF065i	Radial Distribution Function – 065 / weighted by ionization potential
2061	RDF070i	Radial Distribution Function – 070 / weighted by ionization potential
2062	RDF075i	Radial Distribution Function – 075 / weighted by ionization potential
2063	RDF080i	Radial Distribution Function – 080 / weighted by ionization potential
2064	RDF085i	Radial Distribution Function – 085 / weighted by ionization potential
2065	RDF090i	Radial Distribution Function – 090 / weighted by ionization potential
2066	RDF095i	Radial Distribution Function – 095 / weighted by ionization potential
2067	RDF100i	Radial Distribution Function – 100 / weighted by ionization potential
2068	RDF105i	Radial Distribution Function – 105 / weighted by ionization potential
2069	RDF110i	Radial Distribution Function – 110 / weighted by ionization potential
2070	RDF115i	Radial Distribution Function – 115 / weighted by ionization potential
2071	RDF120i	Radial Distribution Function – 120 / weighted by ionization potential
2072	RDF125i	Radial Distribution Function – 125 / weighted by ionization potential
2073	RDF130i	Radial Distribution Function – 130 / weighted by ionization potential
2074	RDF135i	Radial Distribution Function – 135 / weighted by ionization potential
2075	RDF140i	Radial Distribution Function – 140 / weighted by ionization potential
2076	RDF145i	Radial Distribution Function – 145 / weighted by ionization potential
2077	RDF150i	Radial Distribution Function – 150 / weighted by ionization potential
2078	RDF155i	Radial Distribution Function – 155 / weighted by ionization potential
2079	RDF010s	Radial Distribution Function – 010 / weighted by I-state
2080	RDF015s	Radial Distribution Function – 015 / weighted by I-state
2081	RDF020s	Radial Distribution Function – 020 / weighted by I-state
2082	RDF025s	Radial Distribution Function – 025 / weighted by I-state
2083	RDF030s	Radial Distribution Function – 030 / weighted by I-state
2084	RDF035s	Radial Distribution Function – 035 / weighted by I-state
2085	RDF040s	Radial Distribution Function – 040 / weighted by I-state
2086	RDF045s	Radial Distribution Function – 045 / weighted by I-state
2087	RDF050s	Radial Distribution Function – 050 / weighted by I-state
2088	RDF055s	Radial Distribution Function – 055 / weighted by I-state
2089	RDF060s	Radial Distribution Function – 060 / weighted by I-state
2090	RDF065s	Radial Distribution Function – 065 / weighted by I-state
2091	RDF070s	Radial Distribution Function – 070 / weighted by I-state
2092	RDF075s	Radial Distribution Function – 075 / weighted by I-state
2093	RDF080s	Radial Distribution Function – 080 / weighted by I-state
2094	RDF085s	Radial Distribution Function – 085 / weighted by I-state

2095	RDF090s	Radial Distribution Function – 090 / weighted by I-state
2096	RDF095s	Radial Distribution Function – 095 / weighted by I-state
2097	RDF100s	Radial Distribution Function – 100 / weighted by I-state
2098	RDF105s	Radial Distribution Function – 105 / weighted by I-state
2099	RDF110s	Radial Distribution Function – 110 / weighted by I-state
2100	RDF115s	Radial Distribution Function – 115 / weighted by I-state
2101	RDF120s	Radial Distribution Function – 120 / weighted by I-state
2102	RDF125s	Radial Distribution Function – 125 / weighted by I-state
2103	RDF130s	Radial Distribution Function – 130 / weighted by I-state
2104	RDF135s	Radial Distribution Function – 135 / weighted by I-state
2105	RDF140s	Radial Distribution Function – 140 / weighted by I-state
2106	RDF145s	Radial Distribution Function – 145 / weighted by I-state
2107	RDF150s	Radial Distribution Function – 150 / weighted by I-state
2108	RDF155s	Radial Distribution Function – 155 / weighted by I-state

17. 3D-MoRSE descriptors

No.	Name	Description
2109	Mor01u	signal 01 / unweighted
2110	Mor02u	signal 02 / unweighted
2111	Mor03u	signal 03 / unweighted
2112	Mor04u	signal 04 / unweighted
2113	Mor05u	signal 05 / unweighted
2114	Mor06u	signal 06 / unweighted
2115	Mor07u	signal 07 / unweighted
2116	Mor08u	signal 08 / unweighted
2117	Mor09u	signal 09 / unweighted
2118	Mor10u	signal 10 / unweighted
2119	Mor11u	signal 11 / unweighted
2120	Mor12u	signal 12 / unweighted
2121	Mor13u	signal 13 / unweighted
2122	Mor14u	signal 14 / unweighted
2123	Mor15u	signal 15 / unweighted
2124	Mor16u	signal 16 / unweighted
2125	Mor17u	signal 17 / unweighted
2126	Mor18u	signal 18 / unweighted
2127	Mor19u	signal 19 / unweighted
2128	Mor20u	signal 20 / unweighted
2129	Mor21u	signal 21 / unweighted
2130	Mor22u	signal 22 / unweighted
2131	Mor23u	signal 23 / unweighted
2132	Mor24u	signal 24 / unweighted
2133	Mor25u	signal 25 / unweighted

2134	Mor26u	signal 26 / unweighted
2135	Mor27u	signal 27 / unweighted
2136	Mor28u	signal 28 / unweighted
2137	Mor29u	signal 29 / unweighted
2138	Mor30u	signal 30 / unweighted
2139	Mor31u	signal 31 / unweighted
2140	Mor32u	signal 32 / unweighted
2141	Mor01m	signal 01 / weighted by mass
2142	Mor02m	signal 02 / weighted by mass
2143	Mor03m	signal 03 / weighted by mass
2144	Mor04m	signal 04 / weighted by mass
2145	Mor05m	signal 05 / weighted by mass
2146	Mor06m	signal 06 / weighted by mass
2147	Mor07m	signal 07 / weighted by mass
2148	Mor08m	signal 08 / weighted by mass
2149	Mor09m	signal 09 / weighted by mass
2150	Mor10m	signal 10 / weighted by mass
2151	Mor11m	signal 11 / weighted by mass
2152	Mor12m	signal 12 / weighted by mass
2153	Mor13m	signal 13 / weighted by mass
2154	Mor14m	signal 14 / weighted by mass
2155	Mor15m	signal 15 / weighted by mass
2156	Mor16m	signal 16 / weighted by mass
2157	Mor17m	signal 17 / weighted by mass
2158	Mor18m	signal 18 / weighted by mass
2159	Mor19m	signal 19 / weighted by mass
2160	Mor20m	signal 20 / weighted by mass
2161	Mor21m	signal 21 / weighted by mass
2162	Mor22m	signal 22 / weighted by mass
2163	Mor23m	signal 23 / weighted by mass
2164	Mor24m	signal 24 / weighted by mass
2165	Mor25m	signal 25 / weighted by mass
2166	Mor26m	signal 26 / weighted by mass
2167	Mor27m	signal 27 / weighted by mass
2168	Mor28m	signal 28 / weighted by mass
2169	Mor29m	signal 29 / weighted by mass
2170	Mor30m	signal 30 / weighted by mass
2171	Mor31m	signal 31 / weighted by mass
2172	Mor32m	signal 32 / weighted by mass
2173	Mor01v	signal 01 / weighted by van der Waals volume
2174	Mor02v	signal 02 / weighted by van der Waals volume
2175	Mor03v	signal 03 / weighted by van der Waals volume

2176	Mor04v	signal 04 / weighted by van der Waals volume
2177	Mor05v	signal 05 / weighted by van der Waals volume
2178	Mor06v	signal 06 / weighted by van der Waals volume
2179	Mor07v	signal 07 / weighted by van der Waals volume
2180	Mor08v	signal 08 / weighted by van der Waals volume
2181	Mor09v	signal 09 / weighted by van der Waals volume
2182	Mor10v	signal 10 / weighted by van der Waals volume
2183	Mor11v	signal 11 / weighted by van der Waals volume
2184	Mor12v	signal 12 / weighted by van der Waals volume
2185	Mor13v	signal 13 / weighted by van der Waals volume
2186	Mor14v	signal 14 / weighted by van der Waals volume
2187	Mor15v	signal 15 / weighted by van der Waals volume
2188	Mor16v	signal 16 / weighted by van der Waals volume
2189	Mor17v	signal 17 / weighted by van der Waals volume
2190	Mor18v	signal 18 / weighted by van der Waals volume
2191	Mor19v	signal 19 / weighted by van der Waals volume
2192	Mor20v	signal 20 / weighted by van der Waals volume
2193	Mor21v	signal 21 / weighted by van der Waals volume
2194	Mor22v	signal 22 / weighted by van der Waals volume
2195	Mor23v	signal 23 / weighted by van der Waals volume
2196	Mor24v	signal 24 / weighted by van der Waals volume
2197	Mor25v	signal 25 / weighted by van der Waals volume
2198	Mor26v	signal 26 / weighted by van der Waals volume
2199	Mor27v	signal 27 / weighted by van der Waals volume
2200	Mor28v	signal 28 / weighted by van der Waals volume
2201	Mor29v	signal 29 / weighted by van der Waals volume
2202	Mor30v	signal 30 / weighted by van der Waals volume
2203	Mor31v	signal 31 / weighted by van der Waals volume
2204	Mor32v	signal 32 / weighted by van der Waals volume
2205	Mor01e	signal 01 / weighted by Sanderson electronegativity
2206	Mor02e	signal 02 / weighted by Sanderson electronegativity
2207	Mor03e	signal 03 / weighted by Sanderson electronegativity
2208	Mor04e	signal 04 / weighted by Sanderson electronegativity
2209	Mor05e	signal 05 / weighted by Sanderson electronegativity
2210	Mor06e	signal 06 / weighted by Sanderson electronegativity
2211	Mor07e	signal 07 / weighted by Sanderson electronegativity
2212	Mor08e	signal 08 / weighted by Sanderson electronegativity
2213	Mor09e	signal 09 / weighted by Sanderson electronegativity
2214	Mor10e	signal 10 / weighted by Sanderson electronegativity
2215	Mor11e	signal 11 / weighted by Sanderson electronegativity
2216	Mor12e	signal 12 / weighted by Sanderson electronegativity
2217	Mor13e	signal 13 / weighted by Sanderson electronegativity

2218	Mor14e	signal 14 / weighted by Sanderson electronegativity
2219	Mor15e	signal 15 / weighted by Sanderson electronegativity
2220	Mor16e	signal 16 / weighted by Sanderson electronegativity
2221	Mor17e	signal 17 / weighted by Sanderson electronegativity
2222	Mor18e	signal 18 / weighted by Sanderson electronegativity
2223	Mor19e	signal 19 / weighted by Sanderson electronegativity
2224	Mor20e	signal 20 / weighted by Sanderson electronegativity
2225	Mor21e	signal 21 / weighted by Sanderson electronegativity
2226	Mor22e	signal 22 / weighted by Sanderson electronegativity
2227	Mor23e	signal 23 / weighted by Sanderson electronegativity
2228	Mor24e	signal 24 / weighted by Sanderson electronegativity
2229	Mor25e	signal 25 / weighted by Sanderson electronegativity
2230	Mor26e	signal 26 / weighted by Sanderson electronegativity
2231	Mor27e	signal 27 / weighted by Sanderson electronegativity
2232	Mor28e	signal 28 / weighted by Sanderson electronegativity
2233	Mor29e	signal 29 / weighted by Sanderson electronegativity
2234	Mor30e	signal 30 / weighted by Sanderson electronegativity
2235	Mor31e	signal 31 / weighted by Sanderson electronegativity
2236	Mor32e	signal 32 / weighted by Sanderson electronegativity
2237	Mor01p	signal 01 / weighted by polarizability
2238	Mor02p	signal 02 / weighted by polarizability
2239	Mor03p	signal 03 / weighted by polarizability
2240	Mor04p	signal 04 / weighted by polarizability
2241	Mor05p	signal 05 / weighted by polarizability
2242	Mor06p	signal 06 / weighted by polarizability
2243	Mor07p	signal 07 / weighted by polarizability
2244	Mor08p	signal 08 / weighted by polarizability
2245	Mor09p	signal 09 / weighted by polarizability
2246	Mor10p	signal 10 / weighted by polarizability
2247	Mor11p	signal 11 / weighted by polarizability
2248	Mor12p	signal 12 / weighted by polarizability
2249	Mor13p	signal 13 / weighted by polarizability
2250	Mor14p	signal 14 / weighted by polarizability
2251	Mor15p	signal 15 / weighted by polarizability
2252	Mor16p	signal 16 / weighted by polarizability
2253	Mor17p	signal 17 / weighted by polarizability
2254	Mor18p	signal 18 / weighted by polarizability
2255	Mor19p	signal 19 / weighted by polarizability
2256	Mor20p	signal 20 / weighted by polarizability
2257	Mor21p	signal 21 / weighted by polarizability
2258	Mor22p	signal 22 / weighted by polarizability
2259	Mor23p	signal 23 / weighted by polarizability

2260	Mor24p	signal 24 / weighted by polarizability
2261	Mor25p	signal 25 / weighted by polarizability
2262	Mor26p	signal 26 / weighted by polarizability
2263	Mor27p	signal 27 / weighted by polarizability
2264	Mor28p	signal 28 / weighted by polarizability
2265	Mor29p	signal 29 / weighted by polarizability
2266	Mor30p	signal 30 / weighted by polarizability
2267	Mor31p	signal 31 / weighted by polarizability
2268	Mor32p	signal 32 / weighted by polarizability
2269	Mor01i	signal 01 / weighted by ionization potential
2270	Mor02i	signal 02 / weighted by ionization potential
2271	Mor03i	signal 03 / weighted by ionization potential
2272	Mor04i	signal 04 / weighted by ionization potential
2273	Mor05i	signal 05 / weighted by ionization potential
2274	Mor06i	signal 06 / weighted by ionization potential
2275	Mor07i	signal 07 / weighted by ionization potential
2276	Mor08i	signal 08 / weighted by ionization potential
2277	Mor09i	signal 09 / weighted by ionization potential
2278	Mor10i	signal 10 / weighted by ionization potential
2279	Mor11i	signal 11 / weighted by ionization potential
2280	Mor12i	signal 12 / weighted by ionization potential
2281	Mor13i	signal 13 / weighted by ionization potential
2282	Mor14i	signal 14 / weighted by ionization potential
2283	Mor15i	signal 15 / weighted by ionization potential
2284	Mor16i	signal 16 / weighted by ionization potential
2285	Mor17i	signal 17 / weighted by ionization potential
2286	Mor18i	signal 18 / weighted by ionization potential
2287	Mor19i	signal 19 / weighted by ionization potential
2288	Mor20i	signal 20 / weighted by ionization potential
2289	Mor21i	signal 21 / weighted by ionization potential
2290	Mor22i	signal 22 / weighted by ionization potential
2291	Mor23i	signal 23 / weighted by ionization potential
2292	Mor24i	signal 24 / weighted by ionization potential
2293	Mor25i	signal 25 / weighted by ionization potential
2294	Mor26i	signal 26 / weighted by ionization potential
2295	Mor27i	signal 27 / weighted by ionization potential
2296	Mor28i	signal 28 / weighted by ionization potential
2297	Mor29i	signal 29 / weighted by ionization potential
2298	Mor30i	signal 30 / weighted by ionization potential
2299	Mor31i	signal 31 / weighted by ionization potential
2300	Mor32i	signal 32 / weighted by ionization potential
2301	Mor01s	signal 01 / weighted by I-state

2302	Mor02s	signal 02 / weighted by I-state
2303	Mor03s	signal 03 / weighted by I-state
2304	Mor04s	signal 04 / weighted by I-state
2305	Mor05s	signal 05 / weighted by I-state
2306	Mor06s	signal 06 / weighted by I-state
2307	Mor07s	signal 07 / weighted by I-state
2308	Mor08s	signal 08 / weighted by I-state
2309	Mor09s	signal 09 / weighted by I-state
2310	Mor10s	signal 10 / weighted by I-state
2311	Mor11s	signal 11 / weighted by I-state
2312	Mor12s	signal 12 / weighted by I-state
2313	Mor13s	signal 13 / weighted by I-state
2314	Mor14s	signal 14 / weighted by I-state
2315	Mor15s	signal 15 / weighted by I-state
2316	Mor16s	signal 16 / weighted by I-state
2317	Mor17s	signal 17 / weighted by I-state
2318	Mor18s	signal 18 / weighted by I-state
2319	Mor19s	signal 19 / weighted by I-state
2320	Mor20s	signal 20 / weighted by I-state
2321	Mor21s	signal 21 / weighted by I-state
2322	Mor22s	signal 22 / weighted by I-state
2323	Mor23s	signal 23 / weighted by I-state
2324	Mor24s	signal 24 / weighted by I-state
2325	Mor25s	signal 25 / weighted by I-state
2326	Mor26s	signal 26 / weighted by I-state
2327	Mor27s	signal 27 / weighted by I-state
2328	Mor28s	signal 28 / weighted by I-state
2329	Mor29s	signal 29 / weighted by I-state
2330	Mor30s	signal 30 / weighted by I-state
2331	Mor31s	signal 31 / weighted by I-state
2332	Mor32s	signal 32 / weighted by I-state

18. WHIM descriptors

No.	Name	Description
2333	L1u	1st component size directional WHIM index / unweighted
2334	L2u	2nd component size directional WHIM index / unweighted
2335	L3u	3rd component size directional WHIM index / unweighted
2336	P1u	1st component shape directional WHIM index / unweighted
2337	P2u	2nd component shape directional WHIM index / unweighted
2338	G1u	1st component symmetry directional WHIM index / unweighted
2339	G2u	2nd component symmetry directional WHIM index / unweighted
2340	G3u	3rd component symmetry directional WHIM index / unweighted

2341	E1u	1st component accessibility directional WHIM index / unweighted
2342	E2u	2nd component accessibility directional WHIM index / unweighted
2343	E3u	3rd component accessibility directional WHIM index / unweighted
2344	L1m	1st component size directional WHIM index / weighted by mass
2345	L2m	2nd component size directional WHIM index / weighted by mass
2346	L3m	3rd component size directional WHIM index / weighted by mass
2347	P1m	1st component shape directional WHIM index / weighted by mass
2348	P2m	2nd component shape directional WHIM index / weighted by mass
2349	G1m	1st component symmetry directional WHIM index / weighted by mass
2350	G2m	2nd component symmetry directional WHIM index / weighted by mass
2351	G3m	3rd component symmetry directional WHIM index / weighted by mass
2352	E1m	1st component accessibility directional WHIM index / weighted by mass
2353	E2m	2nd component accessibility directional WHIM index / weighted by mass
2354	E3m	3rd component accessibility directional WHIM index / weighted by mass
2355	L1v	1st component size directional WHIM index / weighted by van der Waals volume
2356	L2v	2nd component size directional WHIM index / weighted by van der Waals volume
2357	L3v	3rd component size directional WHIM index / weighted by van der Waals volume
2358	P1v	1st component shape directional WHIM index / weighted by van der Waals volume
2359	P2v	2nd component shape directional WHIM index / weighted by van der Waals volume
2360	G1v	1st component symmetry directional WHIM index / weighted by van der Waals volume
2361	G2v	2nd component symmetry directional WHIM index / weighted by van der Waals volume
2362	G3v	3rd component symmetry directional WHIM index / weighted by van der Waals volume
2363	E1v	1st component accessibility directional WHIM index / weighted by van der Waals volume
2364	E2v	2nd component accessibility directional WHIM index / weighted by van der Waals volume
2365	E3v	3rd component accessibility directional WHIM index / weighted by van der Waals volume
2366	L1e	1st component size directional WHIM index / weighted by Sanderson electronegativity
2367	L2e	2nd component size directional WHIM index / weighted by Sanderson electronegativity
2368	L3e	3rd component size directional WHIM index / weighted by Sanderson electronegativity
2369	P1e	1st component shape directional WHIM index / weighted by Sanderson electronegativity
2370	P2e	2nd component shape directional WHIM index / weighted by Sanderson electronegativity
2371	G1e	1st component symmetry directional WHIM index / weighted by Sanderson electronegativity
2372	G2e	2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity
2373	G3e	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity
2374	E1e	1st component accessibility directional WHIM index / weighted by Sanderson electronegativity
2375	E2e	2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity
2376	E3e	3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity
2377	L1p	1st component size directional WHIM index / weighted by polarizability
2378	L2p	2nd component size directional WHIM index / weighted by polarizability
2379	L3p	3rd component size directional WHIM index / weighted by polarizability
2380	P1p	1st component shape directional WHIM index / weighted by polarizability
2381	P2p	2nd component shape directional WHIM index / weighted by polarizability
2382	G1p	1st component symmetry directional WHIM index / weighted by polarizability

2383	G2p	2nd component symmetry directional WHIM index / weighted by polarizability
2384	G3p	3rd component symmetry directional WHIM index / weighted by polarizability
2385	E1p	1st component accessibility directional WHIM index / weighted by polarizability
2386	E2p	2nd component accessibility directional WHIM index / weighted by polarizability
2387	E3p	3rd component accessibility directional WHIM index / weighted by polarizability
2388	L1i	1st component size directional WHIM index / weighted by ionization potential
2389	L2i	2nd component size directional WHIM index / weighted by ionization potential
2390	L3i	3rd component size directional WHIM index / weighted by ionization potential
2391	P1i	1st component shape directional WHIM index / weighted by ionization potential
2392	P2i	2nd component shape directional WHIM index / weighted by ionization potential
2393	G1i	1st component symmetry directional WHIM index / weighted by ionization potential
2394	G2i	2nd component symmetry directional WHIM index / weighted by ionization potential
2395	G3i	3rd component symmetry directional WHIM index / weighted by ionization potential
2396	E1i	1st component accessibility directional WHIM index / weighted by ionization potential
2397	E2i	2nd component accessibility directional WHIM index / weighted by ionization potential
2398	E3i	3rd component accessibility directional WHIM index / weighted by ionization potential
2399	L1s	1st component size directional WHIM index / weighted by I-state
2400	L2s	2nd component size directional WHIM index / weighted by I-state
2401	L3s	3rd component size directional WHIM index / weighted by I-state
2402	P1s	1st component shape directional WHIM index / weighted by I-state
2403	P2s	2nd component shape directional WHIM index / weighted by I-state
2404	G1s	1st component symmetry directional WHIM index / weighted by I-state
2405	G2s	2nd component symmetry directional WHIM index / weighted by I-state
2406	G3s	3rd component symmetry directional WHIM index / weighted by I-state
2407	E1s	1st component accessibility directional WHIM index / weighted by I-state
2408	E2s	2nd component accessibility directional WHIM index / weighted by I-state
2409	E3s	3rd component accessibility directional WHIM index / weighted by I-state
2410	Tu	T total size index / unweighted
2411	Tm	T total size index / weighted by mass
2412	Tv	T total size index / weighted by van der Waals volume
2413	Te	T total size index / weighted by Sanderson electronegativity
2414	Tp	T total size index / weighted by polarizability
2415	Ti	T total size index / weighted by ionization potential
2416	Ts	T total size index / weighted by I-state
2417	Au	A total size index / unweighted
2418	Am	A total size index / weighted by mass
2419	Av	A total size index / weighted by van der Waals volume
2420	Ae	A total size index / weighted by Sanderson electronegativity
2421	Ap	A total size index / weighted by polarizability
2422	Ai	A total size index / weighted by ionization potential
2423	As	A total size index / weighted by I-state
2424	Gu	total symmetry index / unweighted

2425	Gm	total symmetry index / weighted by mass
2426	Ku	K global shape index / unweighted
2427	Km	K global shape index / weighted by mass
2428	Kv	K global shape index / weighted by van der Waals volume
2429	Ke	K global shape index / weighted by Sanderson electronegativity
2430	Kp	K global shape index / weighted by polarizability
2431	Ki	K global shape index / weighted by ionization potential
2432	Ks	K global shape index / weighted by I-state
2433	Du	D total accessibility index / unweighted
2434	Dm	D total accessibility index / weighted by mass
2435	Dv	D total accessibility index / weighted by van der Waals volume
2436	De	D total accessibility index / weighted by Sanderson electronegativity
2437	Dp	D total accessibility index / weighted by polarizability
2438	Di	D total accessibility index / weighted by ionization potential
2439	Ds	D total accessibility index / weighted by I-state
2440	Vu	V total size index / unweighted
2441	Vm	V total size index / weighted by mass
2442	Vv	V total size index / weighted by van der Waals volume
2443	Ve	V total size index / weighted by Sanderson electronegativity
2444	Vp	V total size index / weighted by polarizability
2445	Vi	V total size index / weighted by ionization potential
2446	Vs	V total size index / weighted by I-state

19. GETAWAY descriptors

No.	Name	Description
2447	ITH	total information content on the leverage equality
2448	ISH	standardized information content on the leverage equality
2449	HIC	mean information content on the leverage magnitude
2450	HGM	geometric mean on the leverage magnitude
2451	H0u	H autocorrelation of lag 0 / unweighted
2452	H1u	H autocorrelation of lag 1 / unweighted
2453	H2u	H autocorrelation of lag 2 / unweighted
2454	H3u	H autocorrelation of lag 3 / unweighted
2455	H4u	H autocorrelation of lag 4 / unweighted
2456	H5u	H autocorrelation of lag 5 / unweighted
2457	H6u	H autocorrelation of lag 6 / unweighted
2458	H7u	H autocorrelation of lag 7 / unweighted
2459	H8u	H autocorrelation of lag 8 / unweighted
2460	HTu	H total index / unweighted
2461	HATS0u	leverage-weighted autocorrelation of lag 0 / unweighted
2462	HATS1u	leverage-weighted autocorrelation of lag 1 / unweighted
2463	HATS2u	leverage-weighted autocorrelation of lag 2 / unweighted

2464	HATS3u	leverage-weighted autocorrelation of lag 3 / unweighted
2465	HATS4u	leverage-weighted autocorrelation of lag 4 / unweighted
2466	HATS5u	leverage-weighted autocorrelation of lag 5 / unweighted
2467	HATS6u	leverage-weighted autocorrelation of lag 6 / unweighted
2468	HATS7u	leverage-weighted autocorrelation of lag 7 / unweighted
2469	HATS8u	leverage-weighted autocorrelation of lag 8 / unweighted
2470	HATSu	leverage-weighted total index / unweighted
2471	H0m	H autocorrelation of lag 0 / weighted by mass
2472	H1m	H autocorrelation of lag 1 / weighted by mass
2473	H2m	H autocorrelation of lag 2 / weighted by mass
2474	H3m	H autocorrelation of lag 3 / weighted by mass
2475	H4m	H autocorrelation of lag 4 / weighted by mass
2476	H5m	H autocorrelation of lag 5 / weighted by mass
2477	H6m	H autocorrelation of lag 6 / weighted by mass
2478	H7m	H autocorrelation of lag 7 / weighted by mass
2479	H8m	H autocorrelation of lag 8 / weighted by mass
2480	HTm	H total index / weighted by mass
2481	HATS0m	leverage-weighted autocorrelation of lag 0 / weighted by mass
2482	HATS1m	leverage-weighted autocorrelation of lag 1 / weighted by mass
2483	HATS2m	leverage-weighted autocorrelation of lag 2 / weighted by mass
2484	HATS3m	leverage-weighted autocorrelation of lag 3 / weighted by mass
2485	HATS4m	leverage-weighted autocorrelation of lag 4 / weighted by mass
2486	HATS5m	leverage-weighted autocorrelation of lag 5 / weighted by mass
2487	HATS6m	leverage-weighted autocorrelation of lag 6 / weighted by mass
2488	HATS7m	leverage-weighted autocorrelation of lag 7 / weighted by mass
2489	HATS8m	leverage-weighted autocorrelation of lag 8 / weighted by mass
2490	HATSm	leverage-weighted total index / weighted by mass
2491	H0v	H autocorrelation of lag 0 / weighted by van der Waals volume
2492	H1v	H autocorrelation of lag 1 / weighted by van der Waals volume
2493	H2v	H autocorrelation of lag 2 / weighted by van der Waals volume
2494	H3v	H autocorrelation of lag 3 / weighted by van der Waals volume
2495	H4v	H autocorrelation of lag 4 / weighted by van der Waals volume
2496	H5v	H autocorrelation of lag 5 / weighted by van der Waals volume
2497	H6v	H autocorrelation of lag 6 / weighted by van der Waals volume
2498	H7v	H autocorrelation of lag 7 / weighted by van der Waals volume
2499	H8v	H autocorrelation of lag 8 / weighted by van der Waals volume
2500	HTv	H total index / weighted by van der Waals volume
2501	HATS0v	leverage-weighted autocorrelation of lag 0 / weighted by van der Waals volume
2502	HATS1v	leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume
2503	HATS2v	leverage-weighted autocorrelation of lag 2 / weighted by van der Waals volume
2504	HATS3v	leverage-weighted autocorrelation of lag 3 / weighted by van der Waals volume
2505	HATS4v	leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume

2506	HATS5v	leverage-weighted autocorrelation of lag 5 / weighted by van der Waals volume
2507	HATS6v	leverage-weighted autocorrelation of lag 6 / weighted by van der Waals volume
2508	HATS7v	leverage-weighted autocorrelation of lag 7 / weighted by van der Waals volume
2509	HATS8v	leverage-weighted autocorrelation of lag 8 / weighted by van der Waals volume
2510	HATSv	leverage-weighted total index / weighted by van der Waals volume
2511	H0e	H autocorrelation of lag 0 / weighted by Sanderson electronegativity
2512	H1e	H autocorrelation of lag 1 / weighted by Sanderson electronegativity
2513	H2e	H autocorrelation of lag 2 / weighted by Sanderson electronegativity
2514	H3e	H autocorrelation of lag 3 / weighted by Sanderson electronegativity
2515	H4e	H autocorrelation of lag 4 / weighted by Sanderson electronegativity
2516	H5e	H autocorrelation of lag 5 / weighted by Sanderson electronegativity
2517	H6e	H autocorrelation of lag 6 / weighted by Sanderson electronegativity
2518	H7e	H autocorrelation of lag 7 / weighted by Sanderson electronegativity
2519	H8e	H autocorrelation of lag 8 / weighted by Sanderson electronegativity
2520	HTe	H total index / weighted by Sanderson electronegativity
2521	HATS0e	leverage-weighted autocorrelation of lag 0 / weighted by Sanderson electronegativity
2522	HATS1e	leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity
2523	HATS2e	leverage-weighted autocorrelation of lag 2 / weighted by Sanderson electronegativity
2524	HATS3e	leverage-weighted autocorrelation of lag 3 / weighted by Sanderson electronegativity
2525	HATS4e	leverage-weighted autocorrelation of lag 4 / weighted by Sanderson electronegativity
2526	HATS5e	leverage-weighted autocorrelation of lag 5 / weighted by Sanderson electronegativity
2527	HATS6e	leverage-weighted autocorrelation of lag 6 / weighted by Sanderson electronegativity
2528	HATS7e	leverage-weighted autocorrelation of lag 7 / weighted by Sanderson electronegativity
2529	HATS8e	leverage-weighted autocorrelation of lag 8 / weighted by Sanderson electronegativity
2530	HATSe	leverage-weighted total index / weighted by Sanderson electronegativity
2531	H0p	H autocorrelation of lag 0 / weighted by polarizability
2532	H1p	H autocorrelation of lag 1 / weighted by polarizability
2533	H2p	H autocorrelation of lag 2 / weighted by polarizability
2534	H3p	H autocorrelation of lag 3 / weighted by polarizability
2535	H4p	H autocorrelation of lag 4 / weighted by polarizability
2536	H5p	H autocorrelation of lag 5 / weighted by polarizability
2537	H6p	H autocorrelation of lag 6 / weighted by polarizability
2538	H7p	H autocorrelation of lag 7 / weighted by polarizability
2539	H8p	H autocorrelation of lag 8 / weighted by polarizability
2540	HTp	H total index / weighted by polarizability
2541	HATS0p	leverage-weighted autocorrelation of lag 0 / weighted by polarizability
2542	HATS1p	leverage-weighted autocorrelation of lag 1 / weighted by polarizability
2543	HATS2p	leverage-weighted autocorrelation of lag 2 / weighted by polarizability
2544	HATS3p	leverage-weighted autocorrelation of lag 3 / weighted by polarizability
2545	HATS4p	leverage-weighted autocorrelation of lag 4 / weighted by polarizability
2546	HATS5p	leverage-weighted autocorrelation of lag 5 / weighted by polarizability
2547	HATS6p	leverage-weighted autocorrelation of lag 6 / weighted by polarizability

2548	HATS7p	leverage-weighted autocorrelation of lag 7 / weighted by polarizability
2549	HATS8p	leverage-weighted autocorrelation of lag 8 / weighted by polarizability
2550	HATSp	leverage-weighted total index / weighted by polarizability
2551	H0i	H autocorrelation of lag 0 / weighted by ionization potential
2552	H1i	H autocorrelation of lag 1 / weighted by ionization potential
2553	H2i	H autocorrelation of lag 2 / weighted by ionization potential
2554	H3i	H autocorrelation of lag 3 / weighted by ionization potential
2555	H4i	H autocorrelation of lag 4 / weighted by ionization potential
2556	H5i	H autocorrelation of lag 5 / weighted by ionization potential
2557	H6i	H autocorrelation of lag 6 / weighted by ionization potential
2558	H7i	H autocorrelation of lag 7 / weighted by ionization potential
2559	H8i	H autocorrelation of lag 8 / weighted by ionization potential
2560	HTi	H total index / weighted by ionization potential
2561	HATS0i	leverage-weighted autocorrelation of lag 0 / weighted by ionization potential
2562	HATS1i	leverage-weighted autocorrelation of lag 1 / weighted by ionization potential
2563	HATS2i	leverage-weighted autocorrelation of lag 2 / weighted by ionization potential
2564	HATS3i	leverage-weighted autocorrelation of lag 3 / weighted by ionization potential
2565	HATS4i	leverage-weighted autocorrelation of lag 4 / weighted by ionization potential
2566	HATS5i	leverage-weighted autocorrelation of lag 5 / weighted by ionization potential
2567	HATS6i	leverage-weighted autocorrelation of lag 6 / weighted by ionization potential
2568	HATS7i	leverage-weighted autocorrelation of lag 7 / weighted by ionization potential
2569	HATS8i	leverage-weighted autocorrelation of lag 8 / weighted by ionization potential
2570	HATSi	leverage-weighted total index / weighted by ionization potential
2571	H0s	H autocorrelation of lag 0 / weighted by I-state
2572	H1s	H autocorrelation of lag 1 / weighted by I-state
2573	H2s	H autocorrelation of lag 2 / weighted by I-state
2574	H3s	H autocorrelation of lag 3 / weighted by I-state
2575	H4s	H autocorrelation of lag 4 / weighted by I-state
2576	H5s	H autocorrelation of lag 5 / weighted by I-state
2577	H6s	H autocorrelation of lag 6 / weighted by I-state
2578	H7s	H autocorrelation of lag 7 / weighted by I-state
2579	H8s	H autocorrelation of lag 8 / weighted by I-state
2580	HTs	H total index / weighted by I-state
2581	HATS0s	leverage-weighted autocorrelation of lag 0 / weighted by I-state
2582	HATS1s	leverage-weighted autocorrelation of lag 1 / weighted by I-state
2583	HATS2s	leverage-weighted autocorrelation of lag 2 / weighted by I-state
2584	HATS3s	leverage-weighted autocorrelation of lag 3 / weighted by I-state
2585	HATS4s	leverage-weighted autocorrelation of lag 4 / weighted by I-state
2586	HATS5s	leverage-weighted autocorrelation of lag 5 / weighted by I-state
2587	HATS6s	leverage-weighted autocorrelation of lag 6 / weighted by I-state
2588	HATS7s	leverage-weighted autocorrelation of lag 7 / weighted by I-state
2589	HATS8s	leverage-weighted autocorrelation of lag 8 / weighted by I-state

2590	HATSs	leverage-weighted total index / weighted by I-state
2591	RCON	Randic-type R matrix connectivity
2592	RARS	R matrix average row sum
2593	REIG	first eigenvalue of the R matrix
2594	R1u	R autocorrelation of lag 1 / unweighted
2595	R2u	R autocorrelation of lag 2 / unweighted
2596	R3u	R autocorrelation of lag 3 / unweighted
2597	R4u	R autocorrelation of lag 4 / unweighted
2598	R5u	R autocorrelation of lag 5 / unweighted
2599	R6u	R autocorrelation of lag 6 / unweighted
2600	R7u	R autocorrelation of lag 7 / unweighted
2601	R8u	R autocorrelation of lag 8 / unweighted
2602	RTu	R total index / unweighted
2603	R1u+	R maximal autocorrelation of lag 1 / unweighted
2604	R2u+	R maximal autocorrelation of lag 2 / unweighted
2605	R3u+	R maximal autocorrelation of lag 3 / unweighted
2606	R4u+	R maximal autocorrelation of lag 4 / unweighted
2607	R5u+	R maximal autocorrelation of lag 5 / unweighted
2608	R6u+	R maximal autocorrelation of lag 6 / unweighted
2609	R7u+	R maximal autocorrelation of lag 7 / unweighted
2610	R8u+	R maximal autocorrelation of lag 8 / unweighted
2611	RTu+	R maximal index / unweighted
2612	R1m	R autocorrelation of lag 1 / weighted by mass
2613	R2m	R autocorrelation of lag 2 / weighted by mass
2614	R3m	R autocorrelation of lag 3 / weighted by mass
2615	R4m	R autocorrelation of lag 4 / weighted by mass
2616	R5m	R autocorrelation of lag 5 / weighted by mass
2617	R6m	R autocorrelation of lag 6 / weighted by mass
2618	R7m	R autocorrelation of lag 7 / weighted by mass
2619	R8m	R autocorrelation of lag 8 / weighted by mass
2620	RTm	R total index / weighted by mass
2621	R1m+	R maximal autocorrelation of lag 1 / weighted by mass
2622	R2m+	R maximal autocorrelation of lag 2 / weighted by mass
2623	R3m+	R maximal autocorrelation of lag 3 / weighted by mass
2624	R4m+	R maximal autocorrelation of lag 4 / weighted by mass
2625	R5m+	R maximal autocorrelation of lag 5 / weighted by mass
2626	R6m+	R maximal autocorrelation of lag 6 / weighted by mass
2627	R7m+	R maximal autocorrelation of lag 7 / weighted by mass
2628	R8m+	R maximal autocorrelation of lag 8 / weighted by mass
2629	RTm+	R maximal index / weighted by mass
2630	R1v	R autocorrelation of lag 1 / weighted by van der Waals volume
2631	R2v	R autocorrelation of lag 2 / weighted by van der Waals volume

2632	R3v	R autocorrelation of lag 3 / weighted by van der Waals volume
2633	R4v	R autocorrelation of lag 4 / weighted by van der Waals volume
2634	R5v	R autocorrelation of lag 5 / weighted by van der Waals volume
2635	R6v	R autocorrelation of lag 6 / weighted by van der Waals volume
2636	R7v	R autocorrelation of lag 7 / weighted by van der Waals volume
2637	R8v	R autocorrelation of lag 8 / weighted by van der Waals volume
2638	RTv	R total index / weighted by van der Waals volume
2639	R1v+	R maximal autocorrelation of lag 1 / weighted by van der Waals volume
2640	R2v+	R maximal autocorrelation of lag 2 / weighted by van der Waals volume
2641	R3v+	R maximal autocorrelation of lag 3 / weighted by van der Waals volume
2642	R4v+	R maximal autocorrelation of lag 4 / weighted by van der Waals volume
2643	R5v+	R maximal autocorrelation of lag 5 / weighted by van der Waals volume
2644	R6v+	R maximal autocorrelation of lag 6 / weighted by van der Waals volume
2645	R7v+	R maximal autocorrelation of lag 7 / weighted by van der Waals volume
2646	R8v+	R maximal autocorrelation of lag 8 / weighted by van der Waals volume
2647	RTv+	R maximal index / weighted by van der Waals volume
2648	R1e	R autocorrelation of lag 1 / weighted by Sanderson electronegativity
2649	R2e	R autocorrelation of lag 2 / weighted by Sanderson electronegativity
2650	R3e	R autocorrelation of lag 3 / weighted by Sanderson electronegativity
2651	R4e	R autocorrelation of lag 4 / weighted by Sanderson electronegativity
2652	R5e	R autocorrelation of lag 5 / weighted by Sanderson electronegativity
2653	R6e	R autocorrelation of lag 6 / weighted by Sanderson electronegativity
2654	R7e	R autocorrelation of lag 7 / weighted by Sanderson electronegativity
2655	R8e	R autocorrelation of lag 8 / weighted by Sanderson electronegativity
2656	RTe	R total index / weighted by Sanderson electronegativity
2657	R1e+	R maximal autocorrelation of lag 1 / weighted by Sanderson electronegativity
2658	R2e+	R maximal autocorrelation of lag 2 / weighted by Sanderson electronegativity
2659	R3e+	R maximal autocorrelation of lag 3 / weighted by Sanderson electronegativity
2660	R4e+	R maximal autocorrelation of lag 4 / weighted by Sanderson electronegativity
2661	R5e+	R maximal autocorrelation of lag 5 / weighted by Sanderson electronegativity
2662	R6e+	R maximal autocorrelation of lag 6 / weighted by Sanderson electronegativity
2663	R7e+	R maximal autocorrelation of lag 7 / weighted by Sanderson electronegativity
2664	R8e+	R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity
2665	RTe+	R maximal index / weighted by Sanderson electronegativity
2666	R1p	R autocorrelation of lag 1 / weighted by polarizability
2667	R2p	R autocorrelation of lag 2 / weighted by polarizability
2668	R3p	R autocorrelation of lag 3 / weighted by polarizability
2669	R4p	R autocorrelation of lag 4 / weighted by polarizability
2670	R5p	R autocorrelation of lag 5 / weighted by polarizability
2671	R6p	R autocorrelation of lag 6 / weighted by polarizability
2672	R7p	R autocorrelation of lag 7 / weighted by polarizability
2673	R8p	R autocorrelation of lag 8 / weighted by polarizability

2674	RTp	R total index / weighted by polarizability
2675	R1p+	R maximal autocorrelation of lag 1 / weighted by polarizability
2676	R2p+	R maximal autocorrelation of lag 2 / weighted by polarizability
2677	R3p+	R maximal autocorrelation of lag 3 / weighted by polarizability
2678	R4p+	R maximal autocorrelation of lag 4 / weighted by polarizability
2679	R5p+	R maximal autocorrelation of lag 5 / weighted by polarizability
2680	R6p+	R maximal autocorrelation of lag 6 / weighted by polarizability
2681	R7p+	R maximal autocorrelation of lag 7 / weighted by polarizability
2682	R8p+	R maximal autocorrelation of lag 8 / weighted by polarizability
2683	RTp+	R maximal index / weighted by polarizability
2684	R1i	R autocorrelation of lag 1 / weighted by ionization potential
2685	R2i	R autocorrelation of lag 2 / weighted by ionization potential
2686	R3i	R autocorrelation of lag 3 / weighted by ionization potential
2687	R4i	R autocorrelation of lag 4 / weighted by ionization potential
2688	R5i	R autocorrelation of lag 5 / weighted by ionization potential
2689	R6i	R autocorrelation of lag 6 / weighted by ionization potential
2690	R7i	R autocorrelation of lag 7 / weighted by ionization potential
2691	R8i	R autocorrelation of lag 8 / weighted by ionization potential
2692	RTi	R total index / weighted by ionization potential
2693	R1i+	R maximal autocorrelation of lag 1 / weighted by ionization potential
2694	R2i+	R maximal autocorrelation of lag 2 / weighted by ionization potential
2695	R3i+	R maximal autocorrelation of lag 3 / weighted by ionization potential
2696	R4i+	R maximal autocorrelation of lag 4 / weighted by ionization potential
2697	R5i+	R maximal autocorrelation of lag 5 / weighted by ionization potential
2698	R6i+	R maximal autocorrelation of lag 6 / weighted by ionization potential
2699	R7i+	R maximal autocorrelation of lag 7 / weighted by ionization potential
2700	R8i+	R maximal autocorrelation of lag 8 / weighted by ionization potential
2701	RTi+	R maximal index / weighted by ionization potential
2702	R1s	R autocorrelation of lag 1 / weighted by I-state
2703	R2s	R autocorrelation of lag 2 / weighted by I-state
2704	R3s	R autocorrelation of lag 3 / weighted by I-state
2705	R4s	R autocorrelation of lag 4 / weighted by I-state
2706	R5s	R autocorrelation of lag 5 / weighted by I-state
2707	R6s	R autocorrelation of lag 6 / weighted by I-state
2708	R7s	R autocorrelation of lag 7 / weighted by I-state
2709	R8s	R autocorrelation of lag 8 / weighted by I-state
2710	RTs	R total index / weighted by I-state
2711	R1s+	R maximal autocorrelation of lag 1 / weighted by I-state
2712	R2s+	R maximal autocorrelation of lag 2 / weighted by I-state
2713	R3s+	R maximal autocorrelation of lag 3 / weighted by I-state
2714	R4s+	R maximal autocorrelation of lag 4 / weighted by I-state
2715	R5s+	R maximal autocorrelation of lag 5 / weighted by I-state

2716	R6s+	R maximal autocorrelation of lag 6 / weighted by I-state
2717	R7s+	R maximal autocorrelation of lag 7 / weighted by I-state
2718	R8s+	R maximal autocorrelation of lag 8 / weighted by I-state
2719	RTs+	R maximal index / weighted by I-state

20. Randic molecular profiles

No.	Name	Description
2720	DP01	molecular profile no. 1
2721	DP02	molecular profile no. 2
2722	DP03	molecular profile no. 3
2723	DP04	molecular profile no. 4
2724	DP05	molecular profile no. 5
2725	DP06	molecular profile no. 6
2726	DP07	molecular profile no. 7
2727	DP08	molecular profile no. 8
2728	DP09	molecular profile no. 9
2729	DP10	molecular profile no. 10
2730	DP11	molecular profile no. 11
2731	DP12	molecular profile no. 12
2732	DP13	molecular profile no. 13
2733	DP14	molecular profile no. 14
2734	DP15	molecular profile no. 15
2735	DP16	molecular profile no. 16
2736	DP17	molecular profile no. 17
2737	DP18	molecular profile no. 18
2738	DP19	molecular profile no. 19
2739	DP20	molecular profile no. 20
2740	SP01	shape profile no. 1
2741	SP02	shape profile no. 2
2742	SP03	shape profile no. 3
2743	SP04	shape profile no. 4
2744	SP05	shape profile no. 5
2745	SP06	shape profile no. 6
2746	SP07	shape profile no. 7
2747	SP08	shape profile no. 8
2748	SP09	shape profile no. 9
2749	SP10	shape profile no. 10
2750	SP11	shape profile no. 11
2751	SP12	shape profile no. 12
2752	SP13	shape profile no. 13
2753	SP14	shape profile no. 14
2754	SP15	shape profile no. 15

2755	SP16	shape profile no. 16
2756	SP17	shape profile no. 17
2757	SP18	shape profile no. 18
2758	SP19	shape profile no. 19
2759	SP20	shape profile no. 20
2760	SHP2	average shape profile index of order 2

21. Functional group counts

No.	Name	Description
2761	nCp	number of terminal primary C(sp3)
2762	nCs	number of total secondary C(sp3)
2763	nCt	number of total tertiary C(sp3)
2764	nCq	number of total quaternary C(sp3)
2765	nCrs	number of ring secondary C(sp3)
2766	nCrt	number of ring tertiary C(sp3)
2767	nCrq	number of ring quaternary C(sp3)
2768	nCar	number of aromatic C(sp2)
2769	nCbH	number of unsubstituted benzene C(sp2)
2770	nCb-	number of substituted benzene C(sp2)
2771	nCconj	number of non-aromatic conjugated C(sp2)
2772	nR=Cp	number of terminal primary C(sp2)
2773	nR=Cs	number of aliphatic secondary C(sp2)
2774	nR=Ct	number of aliphatic tertiary C(sp2)
2775	n=C=	number of allenes groups
2776	nR#CH/X	number of terminal C(sp)
2777	nR#C-	number of non-terminal C(sp)
2778	nROCN	number of cyanates (aliphatic)
2779	nArOCN	number of cyanates (aromatic)
2780	nRNCO	number of isocyanates (aliphatic)
2781	nArNCO	number of isocyanates (aromatic)
2782	nRSCN	number of thiocyanates (aliphatic)
2783	nArSCN	number of thiocyanates (aromatic)
2784	nRNCS	number of isothiocyanates (aliphatic)
2785	nArNCS	number of isothiocyanates (aromatic)
2786	nRCOOH	number of carboxylic acids (aliphatic)
2787	nArCOOH	number of carboxylic acids (aromatic)
2788	nRCOOR	number of esters (aliphatic)
2789	nArCOOR	number of esters (aromatic)
2790	nRCONH2	number of primary amides (aliphatic)
2791	nArCONH2	number of primary amides (aromatic)
2792	nRCONHR	number of secondary amides (aliphatic)
2793	nArCONHR	number of secondary amides (aromatic)

2794	nRCONR2	number of tertiary amides (aliphatic)
2795	nArCONR2	number of tertiary amides (aromatic)
2796	nROCON	number of (thio-) carbamates (aliphatic)
2797	nArOCON	number of (thio-) carbamates (aromatic)
2798	nRCOX	number of acyl halogenides (aliphatic)
2799	nArCOX	number of acyl halogenides (aromatic)
2800	nRCSOH	number of thioacids (aliphatic)
2801	nArCSOH	number of thioacids (aromatic)
2802	nRCSSH	number of dithioacids (aliphatic)
2803	nArCSSH	number of dithioacids (aromatic)
2804	nRCOSR	number of thioesters (aliphatic)
2805	nArCOSR	number of thioesters (aromatic)
2806	nRCSSR	number of dithioesters (aliphatic)
2807	nArCSSR	number of dithioesters (aromatic)
2808	nRCHO	number of aldehydes (aliphatic)
2809	nArCHO	number of aldehydes (aromatic)
2810	nRCO	number of ketones (aliphatic)
2811	nArCO	number of ketones (aromatic)
2812	nCONN	number of urea (-thio) derivatives
2813	nC=O(O)2	number of carbonate (-thio) derivatives
2814	nN=C-N<	number of amidine derivatives
2815	nC(=N)N2	number of guanidine derivatives
2816	nRC=N	number of imines (aliphatic)
2817	nArC=N	number of imines (aromatic)
2818	nRCNO	number of oximes (aliphatic)
2819	nArCNO	number of oximes (aromatic)
2820	nRNH2	number of primary amines (aliphatic)
2821	nArNH2	number of primary amines (aromatic)
2822	nRNHR	number of secondary amines (aliphatic)
2823	nArNHR	number of secondary amines (aromatic)
2824	nRNR2	number of tertiary amines (aliphatic)
2825	nArNR2	number of tertiary amines (aromatic)
2826	nN-N	number of N hydrazines
2827	nN=N	number of N azo-derivatives
2828	nRCN	number of nitriles (aliphatic)
2829	nArCN	number of nitriles (aromatic)
2830	nN+	number of positively charged N
2831	nNq	number of quaternary N
2832	nRNHO	number of hydroxylamines (aliphatic)
2833	nArNHO	number of hydroxylamines (aromatic)
2834	nRNNOx	number of N-nitroso groups (aliphatic)
2835	nArNNOx	number of N-nitroso groups (aromatic)

2836	nRNO	number of nitroso groups (aliphatic)
2837	nArNO	number of nitroso groups (aromatic)
2838	nRNO2	number of nitro groups (aliphatic)
2839	nArNO2	number of nitro groups (aromatic)
2840	nN(CO)2	number of imides (-thio)
2841	nC=N-N<	number of hydrazones
2842	nROH	number of hydroxyl groups
2843	nArOH	number of aromatic hydroxyls
2844	nOHp	number of primary alcohols
2845	nOHs	number of secondary alcohols
2846	nOHt	number of tertiary alcohols
2847	nROR	number of ethers (aliphatic)
2848	nArOR	number of ethers (aromatic)
2849	nROX	number of hypohalogenides (aliphatic)
2850	nArOX	number of hypohalogenides (aromatic)
2851	nO(C=O)2	number of anhydrides (-thio)
2852	nH2O	number of water molecules
2853	nSH	number of thiols
2854	nC=S	number of thioketones
2855	nRSR	number of sulfides
2856	nRSSR	number of disulfides
2857	nSO	number of sulfoxides
2858	nS(=O)2	number of sulfones
2859	nSOH	number of sulfenic (thio-) acids
2860	nSOOH	number of sulfinic (thio-/dithio-) acids
2861	nSO2OH	number of sulfonic (thio-/dithio-) acids
2862	nSO3OH	number of sulfuric (thio-/dithio-) acids
2863	nSO2	number of sulfites (thio-/dithio-)
2864	nSO3	number of sulfonates (thio-/dithio-)
2865	nSO4	number of sulfates (thio-/dithio-)
2866	nSO2N	number of sulfonamides (thio-/dithio-)
2867	nPO3	number of phosphites/thiophosphites
2868	nPO4	number of phosphates/thiophosphates
2869	nPR3	number of phosphanes
2870	nP(=O)O2R	number of phosphonates (thio-)
2871	nP(=O)R3/nPR5	number of phosphoranes (thio-)
2872	nCH2RX	number of CH2RX
2873	nCHR2X	number of CHR2X
2874	nCR3X	number of CR3X
2875	nR=CHX	number of R=CHX
2876	nR=CRX	number of R=CRX
2877	nR#CX	number of R#CX

2878	nCHRX2	number of CHRX2
2879	nCR2X2	number of CR2X2
2880	nR=CX2	number of R=CX2
2881	nCRX3	number of CRX3
2882	nArX	number of X on aromatic ring
2883	nCXr	number of X on ring C(sp3)
2884	nCXr=	number of X on ring C(sp2)
2885	nCconjX	number of X on exo-conjugated C
2886	nAziridines	number of Aziridines
2887	nOxiranes	number of Oxiranes
2888	nThiranes	number of Thiranes
2889	nAzetidines	number of Azetidines
2890	nOxetanes	number of Oxetanes
2891	nThioethanes	number of Thioethanes
2892	nBeta-Lactams	number of Beta-Lactams
2893	nPyrrolidines	number of Pyrrolidines
2894	nOxolanes	number of Oxolanes
2895	ntH-Thiophenes	number of tetrahydro-thiophenes
2896	nPyrroles	number of Pyrroles
2897	nPyrazoles	number of Pyrazoles
2898	nImidazoles	number of Imidazoles
2899	nFuranes	number of Furanes
2900	nThiophenes	number of Thiophenes
2901	nOxazoles	number of Oxazoles
2902	nIsoxazoles	number of Isoxazoles
2903	nThiazoles	number of Thiazoles
2904	nIsothiazoles	number of Isothiazoles
2905	nTriazoles	number of Triazoles
2906	nPyridines	number of Pyridines
2907	nPyridazines	number of Pyridazines
2908	nPyrimidines	number of Pyrimidines
2909	nPyrazines	number of Pyrazines
2910	n135-Triazines	number of 1-3-5-Triazines
2911	n124-Triazines	number of 1-2-4-Triazines
2912	nHDon	number of donor atoms for H-bonds (N and O)
2913	nHAcc	number of acceptor atoms for H-bonds (N,O,F)
2914	nHBonds	number of intramolecular H-bonds (with N,O,F)

22. Atom-centred fragments

No.	Name	Description
2915	C-001	CH3R / CH4
2916	C-002	CH2R2

2917	C-003	CHR3
2918	C-004	CR4
2919	C-005	CH3X
2920	C-006	CH2RX
2921	C-007	CH2X2
2922	C-008	CHR2X
2923	C-009	CHRX2
2924	C-010	CHX3
2925	C-011	CR3X
2926	C-012	CR2X2
2927	C-013	CRX3
2928	C-014	CX4
2929	C-015	
2930	C-016	#NAME?
2931	C-017	
2932	C-018	#NAME?
2933	C-019	#NAME?
2934	C-020	
2935	C-021	#CH
2936	C-022	#CR / R=C=R
2937	C-023	#CX
2938	C-024	R–CH–R
2939	C-025	R–CR–R
2940	C-026	R–CX–R
2941	C-027	R–CH–X
2942	C-028	R–CR–X
2943	C-029	R–CX–X
2944	C-030	X–CH–X
2945	C-031	X–CR–X
2946	C-032	X–CX–X
2947	C-033	R–CH..X
2948	C-034	R–CR..X
2949	C-035	R–CX..X
2950	C-036	Al-CH=X
2951	C-037	Ar-CH=X
2952	C-038	Al-C(=X)-Al
2953	C-039	Ar-C(=X)-R
2954	C-040	R-C(=X)-X / R-C#X / X=C=X
2955	C-041	X-C(=X)-X
2956	C-042	X–CH..X
2957	C-043	X–CR..X
2958	C-044	X–CX..X

2959	H-046	H attached to C0(sp3) no X attached to next C
2960	H-047	H attached to C1(sp3)/C0(sp2)
2961	H-048	H attached to C2(sp3)/C1(sp2)/C0(sp)
2962	H-049	H attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)
2963	H-050	H attached to heteroatom
2964	H-051	H attached to alpha-C
2965	H-052	H attached to C0(sp3) with 1X attached to next C
2966	H-053	H attached to C0(sp3) with 2X attached to next C
2967	H-054	H attached to C0(sp3) with 3X attached to next C
2968	H-055	H attached to C0(sp3) with 4X attached to next C
2969	O-056	alcohol
2970	O-057	phenol / enol / carboxyl OH
2971	O-058	#NAME?
2972	O-059	Al-O-Al
2973	O-060	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X
2974	O-061	O–
2975	O-062	O- (negatively charged)
2976	O-063	R-O-O-R
2977	Se-064	Any-Se-Any
2978	Se-065	#NAME?
2979	N-066	Al-NH2
2980	N-067	Al2-NH
2981	N-068	Al3-N
2982	N-069	Ar-NH2 / X-NH2
2983	N-070	Ar-NH-Al
2984	N-071	Ar-NAl2
2985	N-072	RCO-N< / >N-X=X
2986	N-073	Ar2NH / Ar3N / Ar2N-Al / R..N..R
2987	N-074	R#N / R=N-
2988	N-075	R–N–R / R–N–X
2989	N-076	Ar-NO2 / R–N(–R)–O / RO-NO
2990	N-077	Al-NO2
2991	N-078	Ar-N=X / X-N=X
2992	N-079	N+ (positively charged)
2993	F-081	F attached to C1(sp3)
2994	F-082	F attached to C2(sp3)
2995	F-083	F attached to C3(sp3)
2996	F-084	F attached to C1(sp2)
2997	F-085	F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X
2998	Cl-086	Cl attached to C1(sp3)
2999	Cl-087	Cl attached to C2(sp3)
3000	Cl-088	Cl attached to C3(sp3)

3001	Cl-089	Cl attached to C1(sp2)
3002	Cl-090	Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X
3003	Br-091	Br attached to C1(sp3)
3004	Br-092	Br attached to C2(sp3)
3005	Br-093	Br attached to C3(sp3)
3006	Br-094	Br attached to C1(sp2)
3007	Br-095	Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X
3008	I-096	I attached to C1(sp3)
3009	I-097	I attached to C2(sp3)
3010	I-098	I attached to C3(sp3)
3011	I-099	I attached to C1(sp2)
3012	I-100	I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X
3013	F-101	fluoride ion
3014	Cl-102	chloride ion
3015	Br-103	bromide ion
3016	I-104	iodide ion
3017	S-106	R-SH
3018	S-107	R2S / RS-SR
3019	S-108	R=S
3020	S-109	R-SO-R
3021	S-110	R-SO2-R
3022	Si-111	>Si<
3023	B-112	>B- as in boranes
3024	P-115	P ylids
3025	P-116	R3-P=X
3026	P-117	X3-P=X (phosphate)
3027	P-118	PX3 (phosphite)
3028	P-119	PR3 (phosphine)
3029	P-120	C-P(X)2=X (phosphonate)

23. Atom-type E-state indices

No.	Name	Description
3030	SsCH3	Sum of sCH3 E-states
3031	SdCH2	Sum of dCH2 E-states
3032	SssCH2	Sum of ssCH2 E-states
3033	StCH	Sum of tCH E-states
3034	SdsCH	Sum of dsCH E-states
3035	SaaCH	Sum of aaCH E-states
3036	SsssCH	Sum of sssCH E-states
3037	SddC	Sum of ddC E-states
3038	StsC	Sum of tsC E-states
3039	SdssC	Sum of dssC E-states

3040	SaasC	Sum of aasC E-states
3041	SaaaC	Sum of aaaC E-states
3042	SssssC	Sum of ssssC E-states
3043	SsNH2	Sum of sNH2 E-states
3044	SssNH	Sum of ssNH E-states
3045	SdNH	Sum of dNH E-states
3046	SsssN	Sum of sssN E-states
3047	SdsN	Sum of dsN E-states
3048	SaaN	Sum of aaN E-states
3049	StN	Sum of tN E-states
3050	SsNH3+	Sum of sNH3+ E-states
3051	SssNH2+	Sum of ssNH2+ E-states
3052	SdNH2+	Sum of dNH2+ E-states
3053	SsssNH+	Sum of sssNH+ E-states
3054	SssssN+	Sum of ssssN+ E-states
3055	SddsN	Sum of ddsN E-states
3056	SaadN	Sum of aadN E-states
3057	SaasN	Sum of aasN E-states
3058	SaaNH	Sum of aaNH E-states
3059	SsOH	Sum of sOH E-states
3060	SdO	Sum of dO E-states
3061	SssO	Sum of ssO E-states
3062	SaaO	Sum of aaO E-states
3063	SsPH2	Sum of sPH2 E-states
3064	SssPH	Sum of ssPH E-states
3065	SsssP	Sum of sssP E-states
3066	SdsssP	Sum of dsssP E-states
3067	SddsP	Sum of ddsP E-states
3068	SssssssP	Sum of sssssP E-states
3069	SsSH	Sum of sSH E-states
3070	SdS	Sum of dS E-states
3071	SssS	Sum of ssS E-states
3072	SaaS	Sum of aaS E-states
3073	SdssS	Sum of dssS E-states
3074	SddssS	Sum of ddssS E-states
3075	SssssssS	Sum of ssssssS E-states
3076	SsF	Sum of sF E-states
3077	SsCl	Sum of sCl E-states
3078	SsBr	Sum of sBr E-states
3079	SsI	Sum of sI E-states
3080	SsLi	Sum of sLi E-states
3081	SssBe	Sum of ssBe E-states

3082	SsssBe-	Sum of ssssBe- E-states
3083	SsBH2	Sum of sBH2 E-states
3084	SssBH	Sum of ssBH E-states
3085	SsssB	Sum of sssB E-states
3086	SssssB-	Sum of ssssB- E-states
3087	SsGeH3	Sum of sGeH3 E-states
3088	SssGeH2	Sum of ssGeH2 E-states
3089	SsssGeH	Sum of sssGeH E-states
3090	SssssGe	Sum of ssssGe E-states
3091	SsAsH2	Sum of sAsH2 E-states
3092	SssAsH	Sum of ssAsH E-states
3093	SsssAs	Sum of sssAs E-states
3094	SsssssAs	Sum of sssssAs E-states
3095	SdsssAs	Sum of dsssAs E-states
3096	SddsAs	Sum of ddsAs E-states
3097	SsSeH	Sum of sSeH E-states
3098	SdSe	Sum of dSe E-states
3099	SssSe	Sum of ssSe E-states
3100	SaaSe	Sum of aaSe E-states
3101	SdssSe	Sum of dssSe E-states
3102	SsssssSe	Sum of ssssssSe E-states
3103	SddssSe	Sum of ddssSe E-states
3104	SsSnH3	Sum of sSnH3 E-states
3105	SssSnH2	Sum of ssSnH2 E-states
3106	SsssSnH	Sum of sssSnH E-states
3107	SssssSn	Sum of ssssSn E-states
3108	SsPbH3	Sum of sPbH3 E-states
3109	SssPbH2	Sum of ssPbH2 E-states
3110	SsssPbH	Sum of sssPbH E-states
3111	SssssPb	Sum of ssssPb E-states
3112	SsSiH3	Sum of sSiH3 E-states
3113	SssSiH2	Sum of ssSiH2 E-states
3114	SsssSiH	Sum of sssSiH E-states
3115	SssssSi	Sum of ssssSi E-states
3116	NsCH3	Number of atoms of type sCH3
3117	NdCH2	Number of atoms of type dCH2
3118	NssCH2	Number of atoms of type ssCH2
3119	NtCH	Number of atoms of type tCH
3120	NdsCH	Number of atoms of type dsCH
3121	NaaCH	Number of atoms of type aaCH
3122	NsssCH	Number of atoms of type sssCH
3123	NddC	Number of atoms of type ddC

3124	NtsC	Number of atoms of type tsC
3125	NdssC	Number of atoms of type dssC
3126	NaasC	Number of atoms of type aasC
3127	NaaaC	Number of atoms of type aaaC
3128	NssssC	Number of atoms of type ssssC
3129	NsNH2	Number of atoms of type sNH2
3130	NssNH	Number of atoms of type ssNH
3131	NdNH	Number of atoms of type dNH
3132	NsssN	Number of atoms of type sssN
3133	NdsN	Number of atoms of type dsN
3134	NaaN	Number of atoms of type aaN
3135	NtN	Number of atoms of type tN
3136	NsNH3+	Number of atoms of type sNH3+
3137	NssNH2+	Number of atoms of type ssNH2+
3138	NdNH2+	Number of atoms of type dNH2+
3139	NsssNH+	Number of atoms of type sssNH+
3140	NssssN+	Number of atoms of type ssssN+
3141	NddsN	Number of atoms of type ddsN
3142	NaadN	Number of atoms of type aadN
3143	NaasN	Number of atoms of type aasN
3144	NaaNH	Number of atoms of type aaNH
3145	NsOH	Number of atoms of type sOH
3146	NdO	Number of atoms of type dO
3147	NssO	Number of atoms of type ssO
3148	NaaO	Number of atoms of type aaO
3149	NsPH2	Number of atoms of type sPH2
3150	NssPH	Number of atoms of type ssPH
3151	NsssP	Number of atoms of type sssP
3152	NdsssP	Number of atoms of type dsssP
3153	NddsP	Number of atoms of type ddsP
3154	NssssssP	Number of atoms of type ssssssP
3155	NsSH	Number of atoms of type sSH
3156	NdS	Number of atoms of type dS
3157	NssS	Number of atoms of type ssS
3158	NaaS	Number of atoms of type aaS
3159	NdssS	Number of atoms of type dssS
3160	NddssS	Number of atoms of type ddssS
3161	NsssssssS	Number of atoms of type sssssssS
3162	NsF	Number of atoms of type sF
3163	NsCl	Number of atoms of type sCl
3164	NsBr	Number of atoms of type sBr
3165	NsI	Number of atoms of type sI

3166	NsLi	Number of atoms of type sLi
3167	NssBe	Number of atoms of type ssBe
3168	NssssBe-	Number of atoms of type ssssBe-
3169	NsBH2	Number of atoms of type sBH2
3170	NssBH	Number of atoms of type ssBH
3171	NsssB	Number of atoms of type sssB
3172	NssssB-	Number of atoms of type ssssB-
3173	NsGeH3	Number of atoms of type sGeH3
3174	NssGeH2	Number of atoms of type ssGeH2
3175	NsssGeH	Number of atoms of type sssGeH
3176	NssssGe	Number of atoms of type ssssGe
3177	NsAsH2	Number of atoms of type sAsH2
3178	NssAsH	Number of atoms of type ssAsH
3179	NsssAs	Number of atoms of type sssAs
3180	NssssssAs	Number of atoms of type sssssAs
3181	NdsssAs	Number of atoms of type dsssAs
3182	NddsAs	Number of atoms of type ddsAs
3183	NsSeH	Number of atoms of type sSeH
3184	NdSe	Number of atoms of type dSe
3185	NssSe	Number of atoms of type ssSe
3186	NaaSe	Number of atoms of type aaSe
3187	NdssSe	Number of atoms of type dssSe
3188	NsssssssSe	Number of atoms of type ssssssSe
3189	NddssSe	Number of atoms of type ddssSe
3190	NsSnH3	Number of atoms of type sSnH3
3191	NssSnH2	Number of atoms of type ssSnH2
3192	NsssSnH	Number of atoms of type sssSnH
3193	NssssSn	Number of atoms of type ssssSn
3194	NsPbH3	Number of atoms of type sPbH3
3195	NssPbH2	Number of atoms of type ssPbH2
3196	NsssPbH	Number of atoms of type sssPbH
3197	NssssPb	Number of atoms of type ssssPb
3198	NsSiH3	Number of atoms of type sSiH3
3199	NssSiH2	Number of atoms of type ssSiH2
3200	NsssSiH	Number of atoms of type sssSiH
3201	NssssSi	Number of atoms of type ssssSi
3202	minsCH3	Mimimum sCH3
3203	mindCH2	Mimimum dCH2
3204	minssCH2	Mimimum ssCH2
3205	mintCH	Mimimum tCH
3206	mindsCH	Mimimum dsCH
3207	minaaCH	Mimimum aaCH

3208	minsssCH	Mimimum sssCH
3209	minddC	Mimimum ddC
3210	mintsC	Mimimum tsC
3211	mindssC	Mimimum dssC
3212	minaasC	Mimimum aasC
3213	minaaaC	Mimimum aaaC
3214	minssssC	Mimimum ssssC
3215	minsNH2	Mimimum sNH2
3216	minssNH	Mimimum ssNH
3217	mindNH	Mimimum dNH
3218	minsssN	Mimimum sssN
3219	mindsN	Mimimum dsN
3220	minaaN	Mimimum aaN
3221	mintN	Mimimum tN
3222	minsNH3+	Mimimum sNH3+
3223	minssNH2+	Mimimum ssNH2+
3224	mindNH2+	Mimimum dNH2+
3225	minsssNH+	Mimimum sssNH+
3226	minssssN+	Mimimum ssssN+
3227	minddsN	Mimimum ddsN
3228	minaadN	Mimimum aadN
3229	minaasN	Mimimum aasN
3230	minaaNH	Mimimum aaNH
3231	minsOH	Mimimum sOH
3232	mindO	Mimimum dO
3233	minssO	Mimimum ssO
3234	minaaO	Mimimum aaO
3235	minsPH2	Mimimum sPH2
3236	minssPH	Mimimum ssPH
3237	minsssP	Mimimum sssP
3238	mindsssP	Mimimum dsssP
3239	minddsP	Mimimum ddsP
3240	minsssssP	Mimimum sssssP
3241	minsSH	Mimimum sSH
3242	mindS	Mimimum dS
3243	minssS	Mimimum ssS
3244	minaaS	Mimimum aaS
3245	mindssS	Mimimum dssS
3246	minddssS	Mimimum ddssS
3247	minssssssS	Mimimum ssssssS
3248	minsF	Mimimum sF
3249	minsCl	Mimimum sCl

3250	minsBr	Mimimum sBr
3251	minsI	Mimimum sI
3252	minsLi	Mimimum sLi
3253	minssBe	Mimimum ssBe
3254	minssssBe-	Mimimum ssssBe-
3255	minsBH2	Mimimum sBH2
3256	minssBH	Mimimum ssBH
3257	minsssB	Mimimum sssB
3258	minssssB-	Mimimum ssssB-
3259	minsGeH3	Mimimum sGeH3
3260	minssGeH2	Mimimum ssGeH2
3261	minsssGeH	Mimimum sssGeH
3262	minssssGe	Mimimum ssssGe
3263	minsAsH2	Mimimum sAsH2
3264	minssAsH	Mimimum ssAsH
3265	minsssAs	Mimimum sssAs
3266	minssssssAs	Mimimum sssssAs
3267	mindsssAs	Mimimum dsssAs
3268	minddsAs	Mimimum ddsAs
3269	minsSeH	Mimimum sSeH
3270	mindSe	Mimimum dSe
3271	minssSe	Mimimum ssSe
3272	minaaSe	Mimimum aaSe
3273	mindssSe	Mimimum dssSe
3274	minsssssssSe	Mimimum ssssssSe
3275	minddssSe	Mimimum ddssSe
3276	minsSnH3	Mimimum sSnH3
3277	minssSnH2	Mimimum ssSnH2
3278	minsssSnH	Mimimum sssSnH
3279	minssssSn	Mimimum ssssSn
3280	minsPbH3	Mimimum sPbH3
3281	minssPbH2	Mimimum ssPbH2
3282	minsssPbH	Mimimum sssPbH
3283	minssssPb	Mimimum ssssPb
3284	minsSiH3	Mimimum sSiH3
3285	minssSiH2	Mimimum ssSiH2
3286	minsssSiH	Mimimum sssSiH
3287	minssssSi	Mimimum ssssSi
3288	gmin	Mimimum atom E-state value in a molecule
3289	MaxsCH3	Maximum sCH3
3290	MaxdCH2	Maximum dCH2
3291	MaxssCH2	Maximum ssCH2

3292	MaxtCH	Maximum tCH
3293	MaxdsCH	Maximum dsCH
3294	MaxaaCH	Maximum aaCH
3295	MaxsssCH	Maximum sssCH
3296	MaxddC	Maximum ddC
3297	MaxtsC	Maximum tsC
3298	MaxdssC	Maximum dssC
3299	MaxaasC	Maximum aasC
3300	MaxaaaC	Maximum aaaC
3301	MaxssssC	Maximum ssssC
3302	MaxsNH2	Maximum sNH2
3303	MaxssNH	Maximum ssNH
3304	MaxdNH	Maximum dNH
3305	MaxsssN	Maximum sssN
3306	MaxdsN	Maximum dsN
3307	MaxaaN	Maximum aaN
3308	MaxtN	Maximum tN
3309	MaxsNH3+	Maximum sNH3+
3310	MaxssNH2+	Maximum ssNH2+
3311	MaxdNH2+	Maximum dNH2+
3312	MaxsssNH+	Maximum sssNH+
3313	MaxssssN+	Maximum ssssN+
3314	MaxddsN	Maximum ddsN
3315	MaxaadN	Maximum aadN
3316	MaxaasN	Maximum aasN
3317	MaxaaNH	Maximum aaNH
3318	MaxsOH	Maximum sOH
3319	MaxdO	Maximum dO
3320	MaxssO	Maximum ssO
3321	MaxaaO	Maximum aaO
3322	MaxsPH2	Maximum sPH2
3323	MaxssPH	Maximum ssPH
3324	MaxsssP	Maximum sssP
3325	MaxdsssP	Maximum dsssP
3326	MaxddsP	Maximum ddsP
3327	MaxssssssP	Maximum sssssP
3328	MaxsSH	Maximum sSH
3329	MaxdS	Maximum dS
3330	MaxssS	Maximum ssS
3331	MaxaaS	Maximum aaS
3332	MaxdssS	Maximum dssS
3333	MaxddssS	Maximum ddssS

3334	MaxssssssS	Maximum ssssssS
3335	MaxsF	Maximum sF
3336	MaxsCl	Maximum sCl
3337	MaxsBr	Maximum sBr
3338	MaxsI	Maximum sI
3339	MaxsLi	Maximum sLi
3340	MaxssBe	Maximum ssBe
3341	MaxsssBe-	Maximum ssssBe-
3342	MaxsBH2	Maximum sBH2
3343	MaxssBH	Maximum ssBH
3344	MaxsssB	Maximum sssB
3345	MaxsssB-	Maximum ssssB-
3346	MaxsGeH3	Maximum sGeH3
3347	MaxssGeH2	Maximum ssGeH2
3348	MaxsssGeH	Maximum sssGeH
3349	MaxssssGe	Maximum ssssGe
3350	MaxsAsH2	Maximum sAsH2
3351	MaxssAsH	Maximum ssAsH
3352	MaxsssAs	Maximum sssAs
3353	MaxssssAs	Maximum sssssAs
3354	MaxdsssAs	Maximum dsssAs
3355	MaxddsAs	Maximum ddsAs
3356	MaxsSeH	Maximum sSeH
3357	MaxdSe	Maximum dSe
3358	MaxssSe	Maximum ssSe
3359	MaxaaSe	Maximum aaSe
3360	MaxdssSe	Maximum dssSe
3361	MaxssssssSe	Maximum ssssssSe
3362	MaxddssSe	Maximum ddssSe
3363	MaxsSnH3	Maximum sSnH3
3364	MaxssSnH2	Maximum ssSnH2
3365	MaxsssSnH	Maximum sssSnH
3366	MaxssssSn	Maximum ssssSn
3367	MaxsPbH3	Maximum sPbH3
3368	MaxssPbH2	Maximum ssPbH2
3369	MaxsssPbH	Maximum sssPbH
3370	MaxssssPb	Maximum ssssPb
3371	MaxsSiH3	Maximum sSiH3
3372	MaxssSiH2	Maximum ssSiH2
3373	MaxsssSiH	Maximum sssSiH
3374	MaxssssSi	Maximum ssssSi
3375	gmax	Maximum atom E-state value in a molecule

24. Pharmacophore descriptors

No.	Name	Description
3376	CATS2D_00_DD	CATS2D Donor-Donor at lag 00 (number of H bond donor atoms)
3377	CATS2D_01_DD	CATS2D Donor-Donor at lag 01
3378	CATS2D_02_DD	CATS2D Donor-Donor at lag 02
3379	CATS2D_03_DD	CATS2D Donor-Donor at lag 03
3380	CATS2D_04_DD	CATS2D Donor-Donor at lag 04
3381	CATS2D_05_DD	CATS2D Donor-Donor at lag 05
3382	CATS2D_06_DD	CATS2D Donor-Donor at lag 06
3383	CATS2D_07_DD	CATS2D Donor-Donor at lag 07
3384	CATS2D_08_DD	CATS2D Donor-Donor at lag 08
3385	CATS2D_09_DD	CATS2D Donor-Donor at lag 09
3386	CATS2D_00_DA	CATS2D Donor-Acceptor at lag 00 (number of donor-acceptor atoms)
3387	CATS2D_01_DA	CATS2D Donor-Acceptor at lag 01
3388	CATS2D_02_DA	CATS2D Donor-Acceptor at lag 02
3389	CATS2D_03_DA	CATS2D Donor-Acceptor at lag 03
3390	CATS2D_04_DA	CATS2D Donor-Acceptor at lag 04
3391	CATS2D_05_DA	CATS2D Donor-Acceptor at lag 05
3392	CATS2D_06_DA	CATS2D Donor-Acceptor at lag 06
3393	CATS2D_07_DA	CATS2D Donor-Acceptor at lag 07
3394	CATS2D_08_DA	CATS2D Donor-Acceptor at lag 08
3395	CATS2D_09_DA	CATS2D Donor-Acceptor at lag 09
3396	CATS2D_00_DP	CATS2D Donor-Positive at lag 00 (number of donor-positive atoms)
3397	CATS2D_01_DP	CATS2D Donor-Positive at lag 01
3398	CATS2D_02_DP	CATS2D Donor-Positive at lag 02
3399	CATS2D_03_DP	CATS2D Donor-Positive at lag 03
3400	CATS2D_04_DP	CATS2D Donor-Positive at lag 04
3401	CATS2D_05_DP	CATS2D Donor-Positive at lag 05
3402	CATS2D_06_DP	CATS2D Donor-Positive at lag 06
3403	CATS2D_07_DP	CATS2D Donor-Positive at lag 07
3404	CATS2D_08_DP	CATS2D Donor-Positive at lag 08
3405	CATS2D_09_DP	CATS2D Donor-Positive at lag 09
3406	CATS2D_00_DN	CATS2D Donor-Negative at lag 00 (number of donor-negative atoms)
3407	CATS2D_01_DN	CATS2D Donor-Negative at lag 01
3408	CATS2D_02_DN	CATS2D Donor-Negative at lag 02
3409	CATS2D_03_DN	CATS2D Donor-Negative at lag 03
3410	CATS2D_04_DN	CATS2D Donor-Negative at lag 04
3411	CATS2D_05_DN	CATS2D Donor-Negative at lag 05
3412	CATS2D_06_DN	CATS2D Donor-Negative at lag 06
3413	CATS2D_07_DN	CATS2D Donor-Negative at lag 07
3414	CATS2D_08_DN	CATS2D Donor-Negative at lag 08

3415	CATS2D_09_DN	CATS2D Donor-Negative at lag 09
3416	CATS2D_00_DL	CATS2D Donor-Lipophilic at lag 00 (number of donor-lipohilic atoms)
3417	CATS2D_01_DL	CATS2D Donor-Lipophilic at lag 01
3418	CATS2D_02_DL	CATS2D Donor-Lipophilic at lag 02
3419	CATS2D_03_DL	CATS2D Donor-Lipophilic at lag 03
3420	CATS2D_04_DL	CATS2D Donor-Lipophilic at lag 04
3421	CATS2D_05_DL	CATS2D Donor-Lipophilic at lag 05
3422	CATS2D_06_DL	CATS2D Donor-Lipophilic at lag 06
3423	CATS2D_07_DL	CATS2D Donor-Lipophilic at lag 07
3424	CATS2D_08_DL	CATS2D Donor-Lipophilic at lag 08
3425	CATS2D_09_DL	CATS2D Donor-Lipophilic at lag 09
3426	CATS2D_00_AA	CATS2D Acceptor-Acceptor at lag 00 (number of H bond acceptor atom)
3427	CATS2D_01_AA	CATS2D Acceptor-Acceptor at lag 01
3428	CATS2D_02_AA	CATS2D Acceptor-Acceptor at lag 02
3429	CATS2D_03_AA	CATS2D Acceptor-Acceptor at lag 03
3430	CATS2D_04_AA	CATS2D Acceptor-Acceptor at lag 04
3431	CATS2D_05_AA	CATS2D Acceptor-Acceptor at lag 05
3432	CATS2D_06_AA	CATS2D Acceptor-Acceptor at lag 06
3433	CATS2D_07_AA	CATS2D Acceptor-Acceptor at lag 07
3434	CATS2D_08_AA	CATS2D Acceptor-Acceptor at lag 08
3435	CATS2D_09_AA	CATS2D Acceptor-Acceptor at lag 09
3436	CATS2D_00_AP	CATS2D Acceptor-Positive at lag 00 (number of acceptor-positive atoms)
3437	CATS2D_01_AP	CATS2D Acceptor-Positive at lag 01
3438	CATS2D_02_AP	CATS2D Acceptor-Positive at lag 02
3439	CATS2D_03_AP	CATS2D Acceptor-Positive at lag 03
3440	CATS2D_04_AP	CATS2D Acceptor-Positive at lag 04
3441	CATS2D_05_AP	CATS2D Acceptor-Positive at lag 05
3442	CATS2D_06_AP	CATS2D Acceptor-Positive at lag 06
3443	CATS2D_07_AP	CATS2D Acceptor-Positive at lag 07
3444	CATS2D_08_AP	CATS2D Acceptor-Positive at lag 08
3445	CATS2D_09_AP	CATS2D Acceptor-Positive at lag 09
3446	CATS2D_00_AN	CATS2D Acceptor-Negative at lag 00 (number of acceptor-negative atoms)
3447	CATS2D_01_AN	CATS2D Acceptor-Negative at lag 01
3448	CATS2D_02_AN	CATS2D Acceptor-Negative at lag 02
3449	CATS2D_03_AN	CATS2D Acceptor-Negative at lag 03
3450	CATS2D_04_AN	CATS2D Acceptor-Negative at lag 04
3451	CATS2D_05_AN	CATS2D Acceptor-Negative at lag 05
3452	CATS2D_06_AN	CATS2D Acceptor-Negative at lag 06
3453	CATS2D_07_AN	CATS2D Acceptor-Negative at lag 07
3454	CATS2D_08_AN	CATS2D Acceptor-Negative at lag 08
3455	CATS2D_09_AN	CATS2D Acceptor-Negative at lag 09
3456	CATS2D_00_AL	CATS2D Acceptor-Lipophilic at lag 00 (number of acceptor-lipophilic atoms)

3457	CATS2D_01_AL	CATS2D Acceptor-Lipophilic at lag 01
3458	CATS2D_02_AL	CATS2D Acceptor-Lipophilic at lag 02
3459	CATS2D_03_AL	CATS2D Acceptor-Lipophilic at lag 03
3460	CATS2D_04_AL	CATS2D Acceptor-Lipophilic at lag 04
3461	CATS2D_05_AL	CATS2D Acceptor-Lipophilic at lag 05
3462	CATS2D_06_AL	CATS2D Acceptor-Lipophilic at lag 06
3463	CATS2D_07_AL	CATS2D Acceptor-Lipophilic at lag 07
3464	CATS2D_08_AL	CATS2D Acceptor-Lipophilic at lag 08
3465	CATS2D_09_AL	CATS2D Acceptor-Lipophilic at lag 09
3466	CATS2D_00_PP	CATS2D Positive-Positive at lag 00 (number of positive atoms)
3467	CATS2D_01_PP	CATS2D Positive-Positive at lag 01
3468	CATS2D_02_PP	CATS2D Positive-Positive at lag 02
3469	CATS2D_03_PP	CATS2D Positive-Positive at lag 03
3470	CATS2D_04_PP	CATS2D Positive-Positive at lag 04
3471	CATS2D_05_PP	CATS2D Positive-Positive at lag 05
3472	CATS2D_06_PP	CATS2D Positive-Positive at lag 06
3473	CATS2D_07_PP	CATS2D Positive-Positive at lag 07
3474	CATS2D_08_PP	CATS2D Positive-Positive at lag 08
3475	CATS2D_09_PP	CATS2D Positive-Positive at lag 09
3476	CATS2D_00_PN	CATS2D Positive-Negative at lag 00 (number of positive-negative atoms)
3477	CATS2D_01_PN	CATS2D Positive-Negative at lag 01
3478	CATS2D_02_PN	CATS2D Positive-Negative at lag 02
3479	CATS2D_03_PN	CATS2D Positive-Negative at lag 03
3480	CATS2D_04_PN	CATS2D Positive-Negative at lag 04
3481	CATS2D_05_PN	CATS2D Positive-Negative at lag 05
3482	CATS2D_06_PN	CATS2D Positive-Negative at lag 06
3483	CATS2D_07_PN	CATS2D Positive-Negative at lag 07
3484	CATS2D_08_PN	CATS2D Positive-Negative at lag 08
3485	CATS2D_09_PN	CATS2D Positive-Negative at lag 09
3486	CATS2D_00_PL	CATS2D Positive-Lipophilic at lag 00 (number of positive-lipophilic atoms)
3487	CATS2D_01_PL	CATS2D Positive-Lipophilic at lag 01
3488	CATS2D_02_PL	CATS2D Positive-Lipophilic at lag 02
3489	CATS2D_03_PL	CATS2D Positive-Lipophilic at lag 03
3490	CATS2D_04_PL	CATS2D Positive-Lipophilic at lag 04
3491	CATS2D_05_PL	CATS2D Positive-Lipophilic at lag 05
3492	CATS2D_06_PL	CATS2D Positive-Lipophilic at lag 06
3493	CATS2D_07_PL	CATS2D Positive-Lipophilic at lag 07
3494	CATS2D_08_PL	CATS2D Positive-Lipophilic at lag 08
3495	CATS2D_09_PL	CATS2D Positive-Lipophilic at lag 09
3496	CATS2D_00_NN	CATS2D Negative-Negative at lag 00 (number of negative atoms)
3497	CATS2D_01_NN	CATS2D Negative-Negative at lag 01
3498	CATS2D_02_NN	CATS2D Negative-Negative at lag 02

3499	CATS2D_03_NN	CATS2D Negative-Negative at lag 03
3500	CATS2D_04_NN	CATS2D Negative-Negative at lag 04
3501	CATS2D_05_NN	CATS2D Negative-Negative at lag 05
3502	CATS2D_06_NN	CATS2D Negative-Negative at lag 06
3503	CATS2D_07_NN	CATS2D Negative-Negative at lag 07
3504	CATS2D_08_NN	CATS2D Negative-Negative at lag 08
3505	CATS2D_09_NN	CATS2D Negative-Negative at lag 09
3506	CATS2D_00_NL	CATS2D Negative-Lipophilic at lag 00 (number of negative-lipophilic atoms)
3507	CATS2D_01_NL	CATS2D Negative-Lipophilic at lag 01
3508	CATS2D_02_NL	CATS2D Negative-Lipophilic at lag 02
3509	CATS2D_03_NL	CATS2D Negative-Lipophilic at lag 03
3510	CATS2D_04_NL	CATS2D Negative-Lipophilic at lag 04
3511	CATS2D_05_NL	CATS2D Negative-Lipophilic at lag 05
3512	CATS2D_06_NL	CATS2D Negative-Lipophilic at lag 06
3513	CATS2D_07_NL	CATS2D Negative-Lipophilic at lag 07
3514	CATS2D_08_NL	CATS2D Negative-Lipophilic at lag 08
3515	CATS2D_09_NL	CATS2D Negative-Lipophilic at lag 09
3516	CATS2D_00_LL	CATS2D Lipophilic-Lipophilic at lag 00 (number of lipohilic atoms)
3517	CATS2D_01_LL	CATS2D Lipophilic-Lipophilic at lag 01
3518	CATS2D_02_LL	CATS2D Lipophilic-Lipophilic at lag 02
3519	CATS2D_03_LL	CATS2D Lipophilic-Lipophilic at lag 03
3520	CATS2D_04_LL	CATS2D Lipophilic-Lipophilic at lag 04
3521	CATS2D_05_LL	CATS2D Lipophilic-Lipophilic at lag 05
3522	CATS2D_06_LL	CATS2D Lipophilic-Lipophilic at lag 06
3523	CATS2D_07_LL	CATS2D Lipophilic-Lipophilic at lag 07
3524	CATS2D_08_LL	CATS2D Lipophilic-Lipophilic at lag 08
3525	CATS2D_09_LL	CATS2D Lipophilic-Lipophilic at lag 09
3526	SHED_DD	SHED Donor-Donor
3527	SHED_DA	SHED Donor-Acceptor
3528	SHED_DP	SHED Donor-Positive
3529	SHED_DN	SHED Donor-Negative
3530	SHED_DL	SHED Donor-Lipophilic
3531	SHED_AA	SHED Acceptor-Acceptor
3532	SHED_AP	SHED Acceptor-Positive
3533	SHED_AN	SHED Acceptor-Negative
3534	SHED_AL	SHED Acceptor-Lipophilic
3535	SHED_PP	SHED Positive-Positive
3536	SHED_PN	SHED Positive-Negative
3537	SHED_PL	SHED Positive-Lipophilic
3538	SHED_NN	SHED Negative-Negative
3539	SHED_NL	SHED Negative-Lipophilic
3540	SHED_LL	SHED Lipophilic-Lipophilic

25. 2D Atom Pairs

No.	Name	Description
3541	T(N..N)	sum of topological distances between N..N
3542	T(N..O)	sum of topological distances between N..O
3543	T(N..S)	sum of topological distances between N..S
3544	T(N..P)	sum of topological distances between N..P
3545	T(N..F)	sum of topological distances between N..F
3546	T(N..Cl)	sum of topological distances between N..Cl
3547	T(N..Br)	sum of topological distances between N..Br
3548	T(N..I)	sum of topological distances between N..I
3549	T(O..O)	sum of topological distances between O..O
3550	T(O..S)	sum of topological distances between O..S
3551	T(O..P)	sum of topological distances between O..P
3552	T(O..F)	sum of topological distances between O..F
3553	T(O..Cl)	sum of topological distances between O..Cl
3554	T(O..Br)	sum of topological distances between O..Br
3555	T(O..I)	sum of topological distances between O..I
3556	T(S..S)	sum of topological distances between S..S
3557	T(S..P)	sum of topological distances between S..P
3558	T(S..F)	sum of topological distances between S..F
3559	T(S..Cl)	sum of topological distances between S..Cl
3560	T(S..Br)	sum of topological distances between S..Br
3561	T(S..I)	sum of topological distances between S..I
3562	T(P..P)	sum of topological distances between P..P
3563	T(P..F)	sum of topological distances between P..F
3564	T(P..Cl)	sum of topological distances between P..Cl
3565	T(P..Br)	sum of topological distances between P..Br
3566	T(P..I)	sum of topological distances between P..I
3567	T(F..F)	sum of topological distances between F..F
3568	T(F..Cl)	sum of topological distances between F..Cl
3569	T(F..Br)	sum of topological distances between F..Br
3570	T(F..I)	sum of topological distances between F..I
3571	T(Cl..Cl)	sum of topological distances between Cl..Cl
3572	T(Cl..Br)	sum of topological distances between Cl..Br
3573	T(Cl..I)	sum of topological distances between Cl..I
3574	T(Br..Br)	sum of topological distances between Br..Br
3575	T(Br..I)	sum of topological distances between Br..I
3576	T(I..I)	sum of topological distances between I..I
3577	B01[C-C]	Presence/absence of C – C at topological distance 1
3578	B01[C-N]	Presence/absence of C – N at topological distance 1
3579	B01[C-O]	Presence/absence of C – O at topological distance 1

3580	B01[C-S]	Presence/absence of C – S at topological distance 1
3581	B01[C-P]	Presence/absence of C – P at topological distance 1
3582	B01[C-F]	Presence/absence of C – F at topological distance 1
3583	B01[C-Cl]	Presence/absence of C – Cl at topological distance 1
3584	B01[C-Br]	Presence/absence of C – Br at topological distance 1
3585	B01[C-I]	Presence/absence of C – I at topological distance 1
3586	B01[C-B]	Presence/absence of C – B at topological distance 1
3587	B01[C-Si]	Presence/absence of C – Si at topological distance 1
3588	B01[C-X]	Presence/absence of C – X at topological distance 1
3589	B01[N-N]	Presence/absence of N – N at topological distance 1
3590	B01[N-O]	Presence/absence of N – O at topological distance 1
3591	B01[N-S]	Presence/absence of N – S at topological distance 1
3592	B01[N-P]	Presence/absence of N – P at topological distance 1
3593	B01[N-F]	Presence/absence of N – F at topological distance 1
3594	B01[N-Cl]	Presence/absence of N – Cl at topological distance 1
3595	B01[N-Br]	Presence/absence of N – Br at topological distance 1
3596	B01[N-I]	Presence/absence of N – I at topological distance 1
3597	B01[N-B]	Presence/absence of N – B at topological distance 1
3598	B01[N-Si]	Presence/absence of N – Si at topological distance 1
3599	B01[N-X]	Presence/absence of N – X at topological distance 1
3600	B01[O-O]	Presence/absence of O – O at topological distance 1
3601	B01[O-S]	Presence/absence of O – S at topological distance 1
3602	B01[O-P]	Presence/absence of O – P at topological distance 1
3603	B01[O-F]	Presence/absence of O – F at topological distance 1
3604	B01[O-Cl]	Presence/absence of O – Cl at topological distance 1
3605	B01[O-Br]	Presence/absence of O – Br at topological distance 1
3606	B01[O-I]	Presence/absence of O – I at topological distance 1
3607	B01[O-B]	Presence/absence of O – B at topological distance 1
3608	B01[O-Si]	Presence/absence of O – Si at topological distance 1
3609	B01[O-X]	Presence/absence of O – X at topological distance 1
3610	B01[S-S]	Presence/absence of S – S at topological distance 1
3611	B01[S-P]	Presence/absence of S – P at topological distance 1
3612	B01[S-F]	Presence/absence of S – F at topological distance 1
3613	B01[S-Cl]	Presence/absence of S – Cl at topological distance 1
3614	B01[S-Br]	Presence/absence of S – Br at topological distance 1
3615	B01[S-I]	Presence/absence of S – I at topological distance 1
3616	B01[S-B]	Presence/absence of S – B at topological distance 1
3617	B01[S-Si]	Presence/absence of S – Si at topological distance 1
3618	B01[S-X]	Presence/absence of S – X at topological distance 1
3619	B01[P-P]	Presence/absence of P – P at topological distance 1
3620	B01[P-F]	Presence/absence of P – F at topological distance 1
3621	B01[P-Cl]	Presence/absence of P – Cl at topological distance 1

3622	B01[P-Br]	Presence/absence of P – Br at topological distance 1
3623	B01[P-I]	Presence/absence of P – I at topological distance 1
3624	B01[P-B]	Presence/absence of P – B at topological distance 1
3625	B01[P-Si]	Presence/absence of P – Si at topological distance 1
3626	B01[P-X]	Presence/absence of P – X at topological distance 1
3627	B01[F-F]	Presence/absence of F – F at topological distance 1
3628	B01[F-Cl]	Presence/absence of F – Cl at topological distance 1
3629	B01[F-Br]	Presence/absence of F – Br at topological distance 1
3630	B01[F-I]	Presence/absence of F – I at topological distance 1
3631	B01[F-B]	Presence/absence of F – B at topological distance 1
3632	B01[F-Si]	Presence/absence of F – Si at topological distance 1
3633	B01[F-X]	Presence/absence of F – X at topological distance 1
3634	B01[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 1
3635	B01[Cl-Br]	Presence/absence of Cl – Br at topological distance 1
3636	B01[Cl-I]	Presence/absence of Cl – I at topological distance 1
3637	B01[Cl-B]	Presence/absence of Cl – B at topological distance 1
3638	B01[Cl-Si]	Presence/absence of Cl – Si at topological distance 1
3639	B01[Cl-X]	Presence/absence of Cl – X at topological distance 1
3640	B01[Br-Br]	Presence/absence of Br – Br at topological distance 1
3641	B01[Br-I]	Presence/absence of Br – I at topological distance 1
3642	B01[Br-B]	Presence/absence of Br – B at topological distance 1
3643	B01[Br-Si]	Presence/absence of Br – Si at topological distance 1
3644	B01[Br-X]	Presence/absence of Br – X at topological distance 1
3645	B01[I-I]	Presence/absence of I – I at topological distance 1
3646	B01[I-B]	Presence/absence of I – B at topological distance 1
3647	B01[I-Si]	Presence/absence of I – Si at topological distance 1
3648	B01[I-X]	Presence/absence of I – X at topological distance 1
3649	B01[B-B]	Presence/absence of B – B at topological distance 1
3650	B01[B-Si]	Presence/absence of B – Si at topological distance 1
3651	B01[B-X]	Presence/absence of B – X at topological distance 1
3652	B01[Si-Si]	Presence/absence of Si – Si at topological distance 1
3653	B01[Si-X]	Presence/absence of Si – X at topological distance 1
3654	B01[X-X]	Presence/absence of X – X at topological distance 1
3655	B02[C-C]	Presence/absence of C – C at topological distance 2
3656	B02[C-N]	Presence/absence of C – N at topological distance 2
3657	B02[C-O]	Presence/absence of C – O at topological distance 2
3658	B02[C-S]	Presence/absence of C – S at topological distance 2
3659	B02[C-P]	Presence/absence of C – P at topological distance 2
3660	B02[C-F]	Presence/absence of C – F at topological distance 2
3661	B02[C-Cl]	Presence/absence of C – Cl at topological distance 2
3662	B02[C-Br]	Presence/absence of C – Br at topological distance 2
3663	B02[C-I]	Presence/absence of C – I at topological distance 2

3664	B02[C-B]	Presence/absence of C – B at topological distance 2
3665	B02[C-Si]	Presence/absence of C – Si at topological distance 2
3666	B02[C-X]	Presence/absence of C – X at topological distance 2
3667	B02[N-N]	Presence/absence of N – N at topological distance 2
3668	B02[N-O]	Presence/absence of N – O at topological distance 2
3669	B02[N-S]	Presence/absence of N – S at topological distance 2
3670	B02[N-P]	Presence/absence of N – P at topological distance 2
3671	B02[N-F]	Presence/absence of N – F at topological distance 2
3672	B02[N-Cl]	Presence/absence of N – Cl at topological distance 2
3673	B02[N-Br]	Presence/absence of N – Br at topological distance 2
3674	B02[N-I]	Presence/absence of N – I at topological distance 2
3675	B02[N-B]	Presence/absence of N – B at topological distance 2
3676	B02[N-Si]	Presence/absence of N – Si at topological distance 2
3677	B02[N-X]	Presence/absence of N – X at topological distance 2
3678	B02[O-O]	Presence/absence of O – O at topological distance 2
3679	B02[O-S]	Presence/absence of O – S at topological distance 2
3680	B02[O-P]	Presence/absence of O – P at topological distance 2
3681	B02[O-F]	Presence/absence of O – F at topological distance 2
3682	B02[O-Cl]	Presence/absence of O – Cl at topological distance 2
3683	B02[O-Br]	Presence/absence of O – Br at topological distance 2
3684	B02[O-I]	Presence/absence of O – I at topological distance 2
3685	B02[O-B]	Presence/absence of O – B at topological distance 2
3686	B02[O-Si]	Presence/absence of O – Si at topological distance 2
3687	B02[O-X]	Presence/absence of O – X at topological distance 2
3688	B02[S-S]	Presence/absence of S – S at topological distance 2
3689	B02[S-P]	Presence/absence of S – P at topological distance 2
3690	B02[S-F]	Presence/absence of S – F at topological distance 2
3691	B02[S-Cl]	Presence/absence of S – Cl at topological distance 2
3692	B02[S-Br]	Presence/absence of S – Br at topological distance 2
3693	B02[S-I]	Presence/absence of S – I at topological distance 2
3694	B02[S-B]	Presence/absence of S – B at topological distance 2
3695	B02[S-Si]	Presence/absence of S – Si at topological distance 2
3696	B02[S-X]	Presence/absence of S – X at topological distance 2
3697	B02[P-P]	Presence/absence of P – P at topological distance 2
3698	B02[P-F]	Presence/absence of P – F at topological distance 2
3699	B02[P-Cl]	Presence/absence of P – Cl at topological distance 2
3700	B02[P-Br]	Presence/absence of P – Br at topological distance 2
3701	B02[P-I]	Presence/absence of P – I at topological distance 2
3702	B02[P-B]	Presence/absence of P – B at topological distance 2
3703	B02[P-Si]	Presence/absence of P – Si at topological distance 2
3704	B02[P-X]	Presence/absence of P – X at topological distance 2
3705	B02[F-F]	Presence/absence of F – F at topological distance 2

3706	B02[F-Cl]	Presence/absence of F – Cl at topological distance 2
3707	B02[F-Br]	Presence/absence of F – Br at topological distance 2
3708	B02[F-I]	Presence/absence of F – I at topological distance 2
3709	B02[F-B]	Presence/absence of F – B at topological distance 2
3710	B02[F-Si]	Presence/absence of F – Si at topological distance 2
3711	B02[F-X]	Presence/absence of F – X at topological distance 2
3712	B02[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 2
3713	B02[Cl-Br]	Presence/absence of Cl – Br at topological distance 2
3714	B02[Cl-I]	Presence/absence of Cl – I at topological distance 2
3715	B02[Cl-B]	Presence/absence of Cl – B at topological distance 2
3716	B02[Cl-Si]	Presence/absence of Cl – Si at topological distance 2
3717	B02[Cl-X]	Presence/absence of Cl – X at topological distance 2
3718	B02[Br-Br]	Presence/absence of Br – Br at topological distance 2
3719	B02[Br-I]	Presence/absence of Br – I at topological distance 2
3720	B02[Br-B]	Presence/absence of Br – B at topological distance 2
3721	B02[Br-Si]	Presence/absence of Br – Si at topological distance 2
3722	B02[Br-X]	Presence/absence of Br – X at topological distance 2
3723	B02[I-I]	Presence/absence of I – I at topological distance 2
3724	B02[I-B]	Presence/absence of I – B at topological distance 2
3725	B02[I-Si]	Presence/absence of I – Si at topological distance 2
3726	B02[I-X]	Presence/absence of I – X at topological distance 2
3727	B02[B-B]	Presence/absence of B – B at topological distance 2
3728	B02[B-Si]	Presence/absence of B – Si at topological distance 2
3729	B02[B-X]	Presence/absence of B – X at topological distance 2
3730	B02[Si-Si]	Presence/absence of Si – Si at topological distance 2
3731	B02[Si-X]	Presence/absence of Si – X at topological distance 2
3732	B02[X-X]	Presence/absence of X – X at topological distance 2
3733	B03[C-C]	Presence/absence of C – C at topological distance 3
3734	B03[C-N]	Presence/absence of C – N at topological distance 3
3735	B03[C-O]	Presence/absence of C – O at topological distance 3
3736	B03[C-S]	Presence/absence of C – S at topological distance 3
3737	B03[C-P]	Presence/absence of C – P at topological distance 3
3738	B03[C-F]	Presence/absence of C – F at topological distance 3
3739	B03[C-Cl]	Presence/absence of C – Cl at topological distance 3
3740	B03[C-Br]	Presence/absence of C – Br at topological distance 3
3741	B03[C-I]	Presence/absence of C – I at topological distance 3
3742	B03[C-B]	Presence/absence of C – B at topological distance 3
3743	B03[C-Si]	Presence/absence of C – Si at topological distance 3
3744	B03[C-X]	Presence/absence of C – X at topological distance 3
3745	B03[N-N]	Presence/absence of N – N at topological distance 3
3746	B03[N-O]	Presence/absence of N – O at topological distance 3
3747	B03[N-S]	Presence/absence of N – S at topological distance 3

3748	B03[N-P]	Presence/absence of N – P at topological distance 3
3749	B03[N-F]	Presence/absence of N – F at topological distance 3
3750	B03[N-Cl]	Presence/absence of N – Cl at topological distance 3
3751	B03[N-Br]	Presence/absence of N – Br at topological distance 3
3752	B03[N-I]	Presence/absence of N – I at topological distance 3
3753	B03[N-B]	Presence/absence of N – B at topological distance 3
3754	B03[N-Si]	Presence/absence of N – Si at topological distance 3
3755	B03[N-X]	Presence/absence of N – X at topological distance 3
3756	B03[O-O]	Presence/absence of O – O at topological distance 3
3757	B03[O-S]	Presence/absence of O – S at topological distance 3
3758	B03[O-P]	Presence/absence of O – P at topological distance 3
3759	B03[O-F]	Presence/absence of O – F at topological distance 3
3760	B03[O-Cl]	Presence/absence of O – Cl at topological distance 3
3761	B03[O-Br]	Presence/absence of O – Br at topological distance 3
3762	B03[O-I]	Presence/absence of O – I at topological distance 3
3763	B03[O-B]	Presence/absence of O – B at topological distance 3
3764	B03[O-Si]	Presence/absence of O – Si at topological distance 3
3765	B03[O-X]	Presence/absence of O – X at topological distance 3
3766	B03[S-S]	Presence/absence of S – S at topological distance 3
3767	B03[S-P]	Presence/absence of S – P at topological distance 3
3768	B03[S-F]	Presence/absence of S – F at topological distance 3
3769	B03[S-Cl]	Presence/absence of S – Cl at topological distance 3
3770	B03[S-Br]	Presence/absence of S – Br at topological distance 3
3771	B03[S-I]	Presence/absence of S – I at topological distance 3
3772	B03[S-B]	Presence/absence of S – B at topological distance 3
3773	B03[S-Si]	Presence/absence of S – Si at topological distance 3
3774	B03[S-X]	Presence/absence of S – X at topological distance 3
3775	B03[P-P]	Presence/absence of P – P at topological distance 3
3776	B03[P-F]	Presence/absence of P – F at topological distance 3
3777	B03[P-Cl]	Presence/absence of P – Cl at topological distance 3
3778	B03[P-Br]	Presence/absence of P – Br at topological distance 3
3779	B03[P-I]	Presence/absence of P – I at topological distance 3
3780	B03[P-B]	Presence/absence of P – B at topological distance 3
3781	B03[P-Si]	Presence/absence of P – Si at topological distance 3
3782	B03[P-X]	Presence/absence of P – X at topological distance 3
3783	B03[F-F]	Presence/absence of F – F at topological distance 3
3784	B03[F-Cl]	Presence/absence of F – Cl at topological distance 3
3785	B03[F-Br]	Presence/absence of F – Br at topological distance 3
3786	B03[F-I]	Presence/absence of F – I at topological distance 3
3787	B03[F-B]	Presence/absence of F – B at topological distance 3
3788	B03[F-Si]	Presence/absence of F – Si at topological distance 3
3789	B03[F-X]	Presence/absence of F – X at topological distance 3

3790	B03[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 3
3791	B03[Cl-Br]	Presence/absence of Cl – Br at topological distance 3
3792	B03[Cl-I]	Presence/absence of Cl – I at topological distance 3
3793	B03[Cl-B]	Presence/absence of Cl – B at topological distance 3
3794	B03[Cl-Si]	Presence/absence of Cl – Si at topological distance 3
3795	B03[Cl-X]	Presence/absence of Cl – X at topological distance 3
3796	B03[Br-Br]	Presence/absence of Br – Br at topological distance 3
3797	B03[Br-I]	Presence/absence of Br – I at topological distance 3
3798	B03[Br-B]	Presence/absence of Br – B at topological distance 3
3799	B03[Br-Si]	Presence/absence of Br – Si at topological distance 3
3800	B03[Br-X]	Presence/absence of Br – X at topological distance 3
3801	B03[I-I]	Presence/absence of I – I at topological distance 3
3802	B03[I-B]	Presence/absence of I – B at topological distance 3
3803	B03[I-Si]	Presence/absence of I – Si at topological distance 3
3804	B03[I-X]	Presence/absence of I – X at topological distance 3
3805	B03[B-B]	Presence/absence of B – B at topological distance 3
3806	B03[B-Si]	Presence/absence of B – Si at topological distance 3
3807	B03[B-X]	Presence/absence of B – X at topological distance 3
3808	B03[Si-Si]	Presence/absence of Si – Si at topological distance 3
3809	B03[Si-X]	Presence/absence of Si – X at topological distance 3
3810	B03[X-X]	Presence/absence of X – X at topological distance 3
3811	B04[C-C]	Presence/absence of C – C at topological distance 4
3812	B04[C-N]	Presence/absence of C – N at topological distance 4
3813	B04[C-O]	Presence/absence of C – O at topological distance 4
3814	B04[C-S]	Presence/absence of C – S at topological distance 4
3815	B04[C-P]	Presence/absence of C – P at topological distance 4
3816	B04[C-F]	Presence/absence of C – F at topological distance 4
3817	B04[C-Cl]	Presence/absence of C – Cl at topological distance 4
3818	B04[C-Br]	Presence/absence of C – Br at topological distance 4
3819	B04[C-I]	Presence/absence of C – I at topological distance 4
3820	B04[C-B]	Presence/absence of C – B at topological distance 4
3821	B04[C-Si]	Presence/absence of C – Si at topological distance 4
3822	B04[C-X]	Presence/absence of C – X at topological distance 4
3823	B04[N-N]	Presence/absence of N – N at topological distance 4
3824	B04[N-O]	Presence/absence of N – O at topological distance 4
3825	B04[N-S]	Presence/absence of N – S at topological distance 4
3826	B04[N-P]	Presence/absence of N – P at topological distance 4
3827	B04[N-F]	Presence/absence of N – F at topological distance 4
3828	B04[N-Cl]	Presence/absence of N – Cl at topological distance 4
3829	B04[N-Br]	Presence/absence of N – Br at topological distance 4
3830	B04[N-I]	Presence/absence of N – I at topological distance 4
3831	B04[N-B]	Presence/absence of N – B at topological distance 4

3832	B04[N-Si]	Presence/absence of N – Si at topological distance 4
3833	B04[N-X]	Presence/absence of N – X at topological distance 4
3834	B04[O-O]	Presence/absence of O – O at topological distance 4
3835	B04[O-S]	Presence/absence of O – S at topological distance 4
3836	B04[O-P]	Presence/absence of O – P at topological distance 4
3837	B04[O-F]	Presence/absence of O – F at topological distance 4
3838	B04[O-Cl]	Presence/absence of O – Cl at topological distance 4
3839	B04[O-Br]	Presence/absence of O – Br at topological distance 4
3840	B04[O-I]	Presence/absence of O – I at topological distance 4
3841	B04[O-B]	Presence/absence of O – B at topological distance 4
3842	B04[O-Si]	Presence/absence of O – Si at topological distance 4
3843	B04[O-X]	Presence/absence of O – X at topological distance 4
3844	B04[S-S]	Presence/absence of S – S at topological distance 4
3845	B04[S-P]	Presence/absence of S – P at topological distance 4
3846	B04[S-F]	Presence/absence of S – F at topological distance 4
3847	B04[S-Cl]	Presence/absence of S – Cl at topological distance 4
3848	B04[S-Br]	Presence/absence of S – Br at topological distance 4
3849	B04[S-I]	Presence/absence of S – I at topological distance 4
3850	B04[S-B]	Presence/absence of S – B at topological distance 4
3851	B04[S-Si]	Presence/absence of S – Si at topological distance 4
3852	B04[S-X]	Presence/absence of S – X at topological distance 4
3853	B04[P-P]	Presence/absence of P – P at topological distance 4
3854	B04[P-F]	Presence/absence of P – F at topological distance 4
3855	B04[P-Cl]	Presence/absence of P – Cl at topological distance 4
3856	B04[P-Br]	Presence/absence of P – Br at topological distance 4
3857	B04[P-I]	Presence/absence of P – I at topological distance 4
3858	B04[P-B]	Presence/absence of P – B at topological distance 4
3859	B04[P-Si]	Presence/absence of P – Si at topological distance 4
3860	B04[P-X]	Presence/absence of P – X at topological distance 4
3861	B04[F-F]	Presence/absence of F – F at topological distance 4
3862	B04[F-Cl]	Presence/absence of F – Cl at topological distance 4
3863	B04[F-Br]	Presence/absence of F – Br at topological distance 4
3864	B04[F-I]	Presence/absence of F – I at topological distance 4
3865	B04[F-B]	Presence/absence of F – B at topological distance 4
3866	B04[F-Si]	Presence/absence of F – Si at topological distance 4
3867	B04[F-X]	Presence/absence of F – X at topological distance 4
3868	B04[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 4
3869	B04[Cl-Br]	Presence/absence of Cl – Br at topological distance 4
3870	B04[Cl-I]	Presence/absence of Cl – I at topological distance 4
3871	B04[Cl-B]	Presence/absence of Cl – B at topological distance 4
3872	B04[Cl-Si]	Presence/absence of Cl – Si at topological distance 4
3873	B04[Cl-X]	Presence/absence of Cl – X at topological distance 4

3874	B04[Br-Br]	Presence/absence of Br – Br at topological distance 4
3875	B04[Br-I]	Presence/absence of Br – I at topological distance 4
3876	B04[Br-B]	Presence/absence of Br – B at topological distance 4
3877	B04[Br-Si]	Presence/absence of Br – Si at topological distance 4
3878	B04[Br-X]	Presence/absence of Br – X at topological distance 4
3879	B04[I-I]	Presence/absence of I – I at topological distance 4
3880	B04[I-B]	Presence/absence of I – B at topological distance 4
3881	B04[I-Si]	Presence/absence of I – Si at topological distance 4
3882	B04[I-X]	Presence/absence of I – X at topological distance 4
3883	B04[B-B]	Presence/absence of B – B at topological distance 4
3884	B04[B-Si]	Presence/absence of B – Si at topological distance 4
3885	B04[B-X]	Presence/absence of B – X at topological distance 4
3886	B04[Si-Si]	Presence/absence of Si – Si at topological distance 4
3887	B04[Si-X]	Presence/absence of Si – X at topological distance 4
3888	B04[X-X]	Presence/absence of X – X at topological distance 4
3889	B05[C-C]	Presence/absence of C – C at topological distance 5
3890	B05[C-N]	Presence/absence of C – N at topological distance 5
3891	B05[C-O]	Presence/absence of C – O at topological distance 5
3892	B05[C-S]	Presence/absence of C – S at topological distance 5
3893	B05[C-P]	Presence/absence of C – P at topological distance 5
3894	B05[C-F]	Presence/absence of C – F at topological distance 5
3895	B05[C-Cl]	Presence/absence of C – Cl at topological distance 5
3896	B05[C-Br]	Presence/absence of C – Br at topological distance 5
3897	B05[C-I]	Presence/absence of C – I at topological distance 5
3898	B05[C-B]	Presence/absence of C – B at topological distance 5
3899	B05[C-Si]	Presence/absence of C – Si at topological distance 5
3900	B05[C-X]	Presence/absence of C – X at topological distance 5
3901	B05[N-N]	Presence/absence of N – N at topological distance 5
3902	B05[N-O]	Presence/absence of N – O at topological distance 5
3903	B05[N-S]	Presence/absence of N – S at topological distance 5
3904	B05[N-P]	Presence/absence of N – P at topological distance 5
3905	B05[N-F]	Presence/absence of N – F at topological distance 5
3906	B05[N-Cl]	Presence/absence of N – Cl at topological distance 5
3907	B05[N-Br]	Presence/absence of N – Br at topological distance 5
3908	B05[N-I]	Presence/absence of N – I at topological distance 5
3909	B05[N-B]	Presence/absence of N – B at topological distance 5
3910	B05[N-Si]	Presence/absence of N – Si at topological distance 5
3911	B05[N-X]	Presence/absence of N – X at topological distance 5
3912	B05[O-O]	Presence/absence of O – O at topological distance 5
3913	B05[O-S]	Presence/absence of O – S at topological distance 5
3914	B05[O-P]	Presence/absence of O – P at topological distance 5
3915	B05[O-F]	Presence/absence of O – F at topological distance 5

3916	B05[O-Cl]	Presence/absence of O – Cl at topological distance 5
3917	B05[O-Br]	Presence/absence of O – Br at topological distance 5
3918	B05[O-I]	Presence/absence of O – I at topological distance 5
3919	B05[O-B]	Presence/absence of O – B at topological distance 5
3920	B05[O-Si]	Presence/absence of O – Si at topological distance 5
3921	B05[O-X]	Presence/absence of O – X at topological distance 5
3922	B05[S-S]	Presence/absence of S – S at topological distance 5
3923	B05[S-P]	Presence/absence of S – P at topological distance 5
3924	B05[S-F]	Presence/absence of S – F at topological distance 5
3925	B05[S-Cl]	Presence/absence of S – Cl at topological distance 5
3926	B05[S-Br]	Presence/absence of S – Br at topological distance 5
3927	B05[S-I]	Presence/absence of S – I at topological distance 5
3928	B05[S-B]	Presence/absence of S – B at topological distance 5
3929	B05[S-Si]	Presence/absence of S – Si at topological distance 5
3930	B05[S-X]	Presence/absence of S – X at topological distance 5
3931	B05[P-P]	Presence/absence of P – P at topological distance 5
3932	B05[P-F]	Presence/absence of P – F at topological distance 5
3933	B05[P-Cl]	Presence/absence of P – Cl at topological distance 5
3934	B05[P-Br]	Presence/absence of P – Br at topological distance 5
3935	B05[P-I]	Presence/absence of P – I at topological distance 5
3936	B05[P-B]	Presence/absence of P – B at topological distance 5
3937	B05[P-Si]	Presence/absence of P – Si at topological distance 5
3938	B05[P-X]	Presence/absence of P – X at topological distance 5
3939	B05[F-F]	Presence/absence of F – F at topological distance 5
3940	B05[F-Cl]	Presence/absence of F – Cl at topological distance 5
3941	B05[F-Br]	Presence/absence of F – Br at topological distance 5
3942	B05[F-I]	Presence/absence of F – I at topological distance 5
3943	B05[F-B]	Presence/absence of F – B at topological distance 5
3944	B05[F-Si]	Presence/absence of F – Si at topological distance 5
3945	B05[F-X]	Presence/absence of F – X at topological distance 5
3946	B05[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 5
3947	B05[Cl-Br]	Presence/absence of Cl – Br at topological distance 5
3948	B05[Cl-I]	Presence/absence of Cl – I at topological distance 5
3949	B05[Cl-B]	Presence/absence of Cl – B at topological distance 5
3950	B05[Cl-Si]	Presence/absence of Cl – Si at topological distance 5
3951	B05[Cl-X]	Presence/absence of Cl – X at topological distance 5
3952	B05[Br-Br]	Presence/absence of Br – Br at topological distance 5
3953	B05[Br-I]	Presence/absence of Br – I at topological distance 5
3954	B05[Br-B]	Presence/absence of Br – B at topological distance 5
3955	B05[Br-Si]	Presence/absence of Br – Si at topological distance 5
3956	B05[Br-X]	Presence/absence of Br – X at topological distance 5
3957	B05[I-I]	Presence/absence of I – I at topological distance 5

3958	B05[I-B]	Presence/absence of I – B at topological distance 5
3959	B05[I-Si]	Presence/absence of I – Si at topological distance 5
3960	B05[I-X]	Presence/absence of I – X at topological distance 5
3961	B05[B-B]	Presence/absence of B – B at topological distance 5
3962	B05[B-Si]	Presence/absence of B – Si at topological distance 5
3963	B05[B-X]	Presence/absence of B – X at topological distance 5
3964	B05[Si-Si]	Presence/absence of Si – Si at topological distance 5
3965	B05[Si-X]	Presence/absence of Si – X at topological distance 5
3966	B05[X-X]	Presence/absence of X – X at topological distance 5
3967	B06[C-C]	Presence/absence of C – C at topological distance 6
3968	B06[C-N]	Presence/absence of C – N at topological distance 6
3969	B06[C-O]	Presence/absence of C – O at topological distance 6
3970	B06[C-S]	Presence/absence of C – S at topological distance 6
3971	B06[C-P]	Presence/absence of C – P at topological distance 6
3972	B06[C-F]	Presence/absence of C – F at topological distance 6
3973	B06[C-Cl]	Presence/absence of C – Cl at topological distance 6
3974	B06[C-Br]	Presence/absence of C – Br at topological distance 6
3975	B06[C-I]	Presence/absence of C – I at topological distance 6
3976	B06[C-B]	Presence/absence of C – B at topological distance 6
3977	B06[C-Si]	Presence/absence of C – Si at topological distance 6
3978	B06[C-X]	Presence/absence of C – X at topological distance 6
3979	B06[N-N]	Presence/absence of N – N at topological distance 6
3980	B06[N-O]	Presence/absence of N – O at topological distance 6
3981	B06[N-S]	Presence/absence of N – S at topological distance 6
3982	B06[N-P]	Presence/absence of N – P at topological distance 6
3983	B06[N-F]	Presence/absence of N – F at topological distance 6
3984	B06[N-Cl]	Presence/absence of N – Cl at topological distance 6
3985	B06[N-Br]	Presence/absence of N – Br at topological distance 6
3986	B06[N-I]	Presence/absence of N – I at topological distance 6
3987	B06[N-B]	Presence/absence of N – B at topological distance 6
3988	B06[N-Si]	Presence/absence of N – Si at topological distance 6
3989	B06[N-X]	Presence/absence of N – X at topological distance 6
3990	B06[O-O]	Presence/absence of O – O at topological distance 6
3991	B06[O-S]	Presence/absence of O – S at topological distance 6
3992	B06[O-P]	Presence/absence of O – P at topological distance 6
3993	B06[O-F]	Presence/absence of O – F at topological distance 6
3994	B06[O-Cl]	Presence/absence of O – Cl at topological distance 6
3995	B06[O-Br]	Presence/absence of O – Br at topological distance 6
3996	B06[O-I]	Presence/absence of O – I at topological distance 6
3997	B06[O-B]	Presence/absence of O – B at topological distance 6
3998	B06[O-Si]	Presence/absence of O – Si at topological distance 6
3999	B06[O-X]	Presence/absence of O – X at topological distance 6

4000	B06[S-S]	Presence/absence of S – S at topological distance 6
4001	B06[S-P]	Presence/absence of S – P at topological distance 6
4002	B06[S-F]	Presence/absence of S – F at topological distance 6
4003	B06[S-Cl]	Presence/absence of S – Cl at topological distance 6
4004	B06[S-Br]	Presence/absence of S – Br at topological distance 6
4005	B06[S-I]	Presence/absence of S – I at topological distance 6
4006	B06[S-B]	Presence/absence of S – B at topological distance 6
4007	B06[S-Si]	Presence/absence of S – Si at topological distance 6
4008	B06[S-X]	Presence/absence of S – X at topological distance 6
4009	B06[P-P]	Presence/absence of P – P at topological distance 6
4010	B06[P-F]	Presence/absence of P – F at topological distance 6
4011	B06[P-Cl]	Presence/absence of P – Cl at topological distance 6
4012	B06[P-Br]	Presence/absence of P – Br at topological distance 6
4013	B06[P-I]	Presence/absence of P – I at topological distance 6
4014	B06[P-B]	Presence/absence of P – B at topological distance 6
4015	B06[P-Si]	Presence/absence of P – Si at topological distance 6
4016	B06[P-X]	Presence/absence of P – X at topological distance 6
4017	B06[F-F]	Presence/absence of F – F at topological distance 6
4018	B06[F-Cl]	Presence/absence of F – Cl at topological distance 6
4019	B06[F-Br]	Presence/absence of F – Br at topological distance 6
4020	B06[F-I]	Presence/absence of F – I at topological distance 6
4021	B06[F-B]	Presence/absence of F – B at topological distance 6
4022	B06[F-Si]	Presence/absence of F – Si at topological distance 6
4023	B06[F-X]	Presence/absence of F – X at topological distance 6
4024	B06[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 6
4025	B06[Cl-Br]	Presence/absence of Cl – Br at topological distance 6
4026	B06[Cl-I]	Presence/absence of Cl – I at topological distance 6
4027	B06[Cl-B]	Presence/absence of Cl – B at topological distance 6
4028	B06[Cl-Si]	Presence/absence of Cl – Si at topological distance 6
4029	B06[Cl-X]	Presence/absence of Cl – X at topological distance 6
4030	B06[Br-Br]	Presence/absence of Br – Br at topological distance 6
4031	B06[Br-I]	Presence/absence of Br – I at topological distance 6
4032	B06[Br-B]	Presence/absence of Br – B at topological distance 6
4033	B06[Br-Si]	Presence/absence of Br – Si at topological distance 6
4034	B06[Br-X]	Presence/absence of Br – X at topological distance 6
4035	B06[I-I]	Presence/absence of I – I at topological distance 6
4036	B06[I-B]	Presence/absence of I – B at topological distance 6
4037	B06[I-Si]	Presence/absence of I – Si at topological distance 6
4038	B06[I-X]	Presence/absence of I – X at topological distance 6
4039	B06[B-B]	Presence/absence of B – B at topological distance 6
4040	B06[B-Si]	Presence/absence of B – Si at topological distance 6
4041	B06[B-X]	Presence/absence of B – X at topological distance 6

4042	B06[Si-Si]	Presence/absence of Si – Si at topological distance 6
4043	B06[Si-X]	Presence/absence of Si – X at topological distance 6
4044	B06[X-X]	Presence/absence of X – X at topological distance 6
4045	B07[C-C]	Presence/absence of C – C at topological distance 7
4046	B07[C-N]	Presence/absence of C – N at topological distance 7
4047	B07[C-O]	Presence/absence of C – O at topological distance 7
4048	B07[C-S]	Presence/absence of C – S at topological distance 7
4049	B07[C-P]	Presence/absence of C – P at topological distance 7
4050	B07[C-F]	Presence/absence of C – F at topological distance 7
4051	B07[C-Cl]	Presence/absence of C – Cl at topological distance 7
4052	B07[C-Br]	Presence/absence of C – Br at topological distance 7
4053	B07[C-I]	Presence/absence of C – I at topological distance 7
4054	B07[C-B]	Presence/absence of C – B at topological distance 7
4055	B07[C-Si]	Presence/absence of C – Si at topological distance 7
4056	B07[C-X]	Presence/absence of C – X at topological distance 7
4057	B07[N-N]	Presence/absence of N – N at topological distance 7
4058	B07[N-O]	Presence/absence of N – O at topological distance 7
4059	B07[N-S]	Presence/absence of N – S at topological distance 7
4060	B07[N-P]	Presence/absence of N – P at topological distance 7
4061	B07[N-F]	Presence/absence of N – F at topological distance 7
4062	B07[N-Cl]	Presence/absence of N – Cl at topological distance 7
4063	B07[N-Br]	Presence/absence of N – Br at topological distance 7
4064	B07[N-I]	Presence/absence of N – I at topological distance 7
4065	B07[N-B]	Presence/absence of N – B at topological distance 7
4066	B07[N-Si]	Presence/absence of N – Si at topological distance 7
4067	B07[N-X]	Presence/absence of N – X at topological distance 7
4068	B07[O-O]	Presence/absence of O – O at topological distance 7
4069	B07[O-S]	Presence/absence of O – S at topological distance 7
4070	B07[O-P]	Presence/absence of O – P at topological distance 7
4071	B07[O-F]	Presence/absence of O – F at topological distance 7
4072	B07[O-Cl]	Presence/absence of O – Cl at topological distance 7
4073	B07[O-Br]	Presence/absence of O – Br at topological distance 7
4074	B07[O-I]	Presence/absence of O – I at topological distance 7
4075	B07[O-B]	Presence/absence of O – B at topological distance 7
4076	B07[O-Si]	Presence/absence of O – Si at topological distance 7
4077	B07[O-X]	Presence/absence of O – X at topological distance 7
4078	B07[S-S]	Presence/absence of S – S at topological distance 7
4079	B07[S-P]	Presence/absence of S – P at topological distance 7
4080	B07[S-F]	Presence/absence of S – F at topological distance 7
4081	B07[S-Cl]	Presence/absence of S – Cl at topological distance 7
4082	B07[S-Br]	Presence/absence of S – Br at topological distance 7
4083	B07[S-I]	Presence/absence of S – I at topological distance 7

4084	B07[S-B]	Presence/absence of S – B at topological distance 7
4085	B07[S-Si]	Presence/absence of S – Si at topological distance 7
4086	B07[S-X]	Presence/absence of S – X at topological distance 7
4087	B07[P-P]	Presence/absence of P – P at topological distance 7
4088	B07[P-F]	Presence/absence of P – F at topological distance 7
4089	B07[P-Cl]	Presence/absence of P – Cl at topological distance 7
4090	B07[P-Br]	Presence/absence of P – Br at topological distance 7
4091	B07[P-I]	Presence/absence of P – I at topological distance 7
4092	B07[P-B]	Presence/absence of P – B at topological distance 7
4093	B07[P-Si]	Presence/absence of P – Si at topological distance 7
4094	B07[P-X]	Presence/absence of P – X at topological distance 7
4095	B07[F-F]	Presence/absence of F – F at topological distance 7
4096	B07[F-Cl]	Presence/absence of F – Cl at topological distance 7
4097	B07[F-Br]	Presence/absence of F – Br at topological distance 7
4098	B07[F-I]	Presence/absence of F – I at topological distance 7
4099	B07[F-B]	Presence/absence of F – B at topological distance 7
4100	B07[F-Si]	Presence/absence of F – Si at topological distance 7
4101	B07[F-X]	Presence/absence of F – X at topological distance 7
4102	B07[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 7
4103	B07[Cl-Br]	Presence/absence of Cl – Br at topological distance 7
4104	B07[Cl-I]	Presence/absence of Cl – I at topological distance 7
4105	B07[Cl-B]	Presence/absence of Cl – B at topological distance 7
4106	B07[Cl-Si]	Presence/absence of Cl – Si at topological distance 7
4107	B07[Cl-X]	Presence/absence of Cl – X at topological distance 7
4108	B07[Br-Br]	Presence/absence of Br – Br at topological distance 7
4109	B07[Br-I]	Presence/absence of Br – I at topological distance 7
4110	B07[Br-B]	Presence/absence of Br – B at topological distance 7
4111	B07[Br-Si]	Presence/absence of Br – Si at topological distance 7
4112	B07[Br-X]	Presence/absence of Br – X at topological distance 7
4113	B07[I-I]	Presence/absence of I – I at topological distance 7
4114	B07[I-B]	Presence/absence of I – B at topological distance 7
4115	B07[I-Si]	Presence/absence of I – Si at topological distance 7
4116	B07[I-X]	Presence/absence of I – X at topological distance 7
4117	B07[B-B]	Presence/absence of B – B at topological distance 7
4118	B07[B-Si]	Presence/absence of B – Si at topological distance 7
4119	B07[B-X]	Presence/absence of B – X at topological distance 7
4120	B07[Si-Si]	Presence/absence of Si – Si at topological distance 7
4121	B07[Si-X]	Presence/absence of Si – X at topological distance 7
4122	B07[X-X]	Presence/absence of X – X at topological distance 7
4123	B08[C-C]	Presence/absence of C – C at topological distance 8
4124	B08[C-N]	Presence/absence of C – N at topological distance 8
4125	B08[C-O]	Presence/absence of C – O at topological distance 8

4126	B08[C-S]	Presence/absence of C – S at topological distance 8
4127	B08[C-P]	Presence/absence of C – P at topological distance 8
4128	B08[C-F]	Presence/absence of C – F at topological distance 8
4129	B08[C-Cl]	Presence/absence of C – Cl at topological distance 8
4130	B08[C-Br]	Presence/absence of C – Br at topological distance 8
4131	B08[C-I]	Presence/absence of C – I at topological distance 8
4132	B08[C-B]	Presence/absence of C – B at topological distance 8
4133	B08[C-Si]	Presence/absence of C – Si at topological distance 8
4134	B08[C-X]	Presence/absence of C – X at topological distance 8
4135	B08[N-N]	Presence/absence of N – N at topological distance 8
4136	B08[N-O]	Presence/absence of N – O at topological distance 8
4137	B08[N-S]	Presence/absence of N – S at topological distance 8
4138	B08[N-P]	Presence/absence of N – P at topological distance 8
4139	B08[N-F]	Presence/absence of N – F at topological distance 8
4140	B08[N-Cl]	Presence/absence of N – Cl at topological distance 8
4141	B08[N-Br]	Presence/absence of N – Br at topological distance 8
4142	B08[N-I]	Presence/absence of N – I at topological distance 8
4143	B08[N-B]	Presence/absence of N – B at topological distance 8
4144	B08[N-Si]	Presence/absence of N – Si at topological distance 8
4145	B08[N-X]	Presence/absence of N – X at topological distance 8
4146	B08[O-O]	Presence/absence of O – O at topological distance 8
4147	B08[O-S]	Presence/absence of O – S at topological distance 8
4148	B08[O-P]	Presence/absence of O – P at topological distance 8
4149	B08[O-F]	Presence/absence of O – F at topological distance 8
4150	B08[O-Cl]	Presence/absence of O – Cl at topological distance 8
4151	B08[O-Br]	Presence/absence of O – Br at topological distance 8
4152	B08[O-I]	Presence/absence of O – I at topological distance 8
4153	B08[O-B]	Presence/absence of O – B at topological distance 8
4154	B08[O-Si]	Presence/absence of O – Si at topological distance 8
4155	B08[O-X]	Presence/absence of O – X at topological distance 8
4156	B08[S-S]	Presence/absence of S – S at topological distance 8
4157	B08[S-P]	Presence/absence of S – P at topological distance 8
4158	B08[S-F]	Presence/absence of S – F at topological distance 8
4159	B08[S-Cl]	Presence/absence of S – Cl at topological distance 8
4160	B08[S-Br]	Presence/absence of S – Br at topological distance 8
4161	B08[S-I]	Presence/absence of S – I at topological distance 8
4162	B08[S-B]	Presence/absence of S – B at topological distance 8
4163	B08[S-Si]	Presence/absence of S – Si at topological distance 8
4164	B08[S-X]	Presence/absence of S – X at topological distance 8
4165	B08[P-P]	Presence/absence of P – P at topological distance 8
4166	B08[P-F]	Presence/absence of P – F at topological distance 8
4167	B08[P-Cl]	Presence/absence of P – Cl at topological distance 8

4168	B08[P-Br]	Presence/absence of P – Br at topological distance 8
4169	B08[P-I]	Presence/absence of P – I at topological distance 8
4170	B08[P-B]	Presence/absence of P – B at topological distance 8
4171	B08[P-Si]	Presence/absence of P – Si at topological distance 8
4172	B08[P-X]	Presence/absence of P – X at topological distance 8
4173	B08[F-F]	Presence/absence of F – F at topological distance 8
4174	B08[F-Cl]	Presence/absence of F – Cl at topological distance 8
4175	B08[F-Br]	Presence/absence of F – Br at topological distance 8
4176	B08[F-I]	Presence/absence of F – I at topological distance 8
4177	B08[F-B]	Presence/absence of F – B at topological distance 8
4178	B08[F-Si]	Presence/absence of F – Si at topological distance 8
4179	B08[F-X]	Presence/absence of F – X at topological distance 8
4180	B08[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 8
4181	B08[Cl-Br]	Presence/absence of Cl – Br at topological distance 8
4182	B08[Cl-I]	Presence/absence of Cl – I at topological distance 8
4183	B08[Cl-B]	Presence/absence of Cl – B at topological distance 8
4184	B08[Cl-Si]	Presence/absence of Cl – Si at topological distance 8
4185	B08[Cl-X]	Presence/absence of Cl – X at topological distance 8
4186	B08[Br-Br]	Presence/absence of Br – Br at topological distance 8
4187	B08[Br-I]	Presence/absence of Br – I at topological distance 8
4188	B08[Br-B]	Presence/absence of Br – B at topological distance 8
4189	B08[Br-Si]	Presence/absence of Br – Si at topological distance 8
4190	B08[Br-X]	Presence/absence of Br – X at topological distance 8
4191	B08[I-I]	Presence/absence of I – I at topological distance 8
4192	B08[I-B]	Presence/absence of I – B at topological distance 8
4193	B08[I-Si]	Presence/absence of I – Si at topological distance 8
4194	B08[I-X]	Presence/absence of I – X at topological distance 8
4195	B08[B-B]	Presence/absence of B – B at topological distance 8
4196	B08[B-Si]	Presence/absence of B – Si at topological distance 8
4197	B08[B-X]	Presence/absence of B – X at topological distance 8
4198	B08[Si-Si]	Presence/absence of Si – Si at topological distance 8
4199	B08[Si-X]	Presence/absence of Si – X at topological distance 8
4200	B08[X-X]	Presence/absence of X – X at topological distance 8
4201	B09[C-C]	Presence/absence of C – C at topological distance 9
4202	B09[C-N]	Presence/absence of C – N at topological distance 9
4203	B09[C-O]	Presence/absence of C – O at topological distance 9
4204	B09[C-S]	Presence/absence of C – S at topological distance 9
4205	B09[C-P]	Presence/absence of C – P at topological distance 9
4206	B09[C-F]	Presence/absence of C – F at topological distance 9
4207	B09[C-Cl]	Presence/absence of C – Cl at topological distance 9
4208	B09[C-Br]	Presence/absence of C – Br at topological distance 9
4209	B09[C-I]	Presence/absence of C – I at topological distance 9

4210	B09[C-B]	Presence/absence of C – B at topological distance 9
4211	B09[C-Si]	Presence/absence of C – Si at topological distance 9
4212	B09[C-X]	Presence/absence of C – X at topological distance 9
4213	B09[N-N]	Presence/absence of N – N at topological distance 9
4214	B09[N-O]	Presence/absence of N – O at topological distance 9
4215	B09[N-S]	Presence/absence of N – S at topological distance 9
4216	B09[N-P]	Presence/absence of N – P at topological distance 9
4217	B09[N-F]	Presence/absence of N – F at topological distance 9
4218	B09[N-Cl]	Presence/absence of N – Cl at topological distance 9
4219	B09[N-Br]	Presence/absence of N – Br at topological distance 9
4220	B09[N-I]	Presence/absence of N – I at topological distance 9
4221	B09[N-B]	Presence/absence of N – B at topological distance 9
4222	B09[N-Si]	Presence/absence of N – Si at topological distance 9
4223	B09[N-X]	Presence/absence of N – X at topological distance 9
4224	B09[O-O]	Presence/absence of O – O at topological distance 9
4225	B09[O-S]	Presence/absence of O – S at topological distance 9
4226	B09[O-P]	Presence/absence of O – P at topological distance 9
4227	B09[O-F]	Presence/absence of O – F at topological distance 9
4228	B09[O-Cl]	Presence/absence of O – Cl at topological distance 9
4229	B09[O-Br]	Presence/absence of O – Br at topological distance 9
4230	B09[O-I]	Presence/absence of O – I at topological distance 9
4231	B09[O-B]	Presence/absence of O – B at topological distance 9
4232	B09[O-Si]	Presence/absence of O – Si at topological distance 9
4233	B09[O-X]	Presence/absence of O – X at topological distance 9
4234	B09[S-S]	Presence/absence of S – S at topological distance 9
4235	B09[S-P]	Presence/absence of S – P at topological distance 9
4236	B09[S-F]	Presence/absence of S – F at topological distance 9
4237	B09[S-Cl]	Presence/absence of S – Cl at topological distance 9
4238	B09[S-Br]	Presence/absence of S – Br at topological distance 9
4239	B09[S-I]	Presence/absence of S – I at topological distance 9
4240	B09[S-B]	Presence/absence of S – B at topological distance 9
4241	B09[S-Si]	Presence/absence of S – Si at topological distance 9
4242	B09[S-X]	Presence/absence of S – X at topological distance 9
4243	B09[P-P]	Presence/absence of P – P at topological distance 9
4244	B09[P-F]	Presence/absence of P – F at topological distance 9
4245	B09[P-Cl]	Presence/absence of P – Cl at topological distance 9
4246	B09[P-Br]	Presence/absence of P – Br at topological distance 9
4247	B09[P-I]	Presence/absence of P – I at topological distance 9
4248	B09[P-B]	Presence/absence of P – B at topological distance 9
4249	B09[P-Si]	Presence/absence of P – Si at topological distance 9
4250	B09[P-X]	Presence/absence of P – X at topological distance 9
4251	B09[F-F]	Presence/absence of F – F at topological distance 9

4252	B09[F-Cl]	Presence/absence of F – Cl at topological distance 9
4253	B09[F-Br]	Presence/absence of F – Br at topological distance 9
4254	B09[F-I]	Presence/absence of F – I at topological distance 9
4255	B09[F-B]	Presence/absence of F – B at topological distance 9
4256	B09[F-Si]	Presence/absence of F – Si at topological distance 9
4257	B09[F-X]	Presence/absence of F – X at topological distance 9
4258	B09[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 9
4259	B09[Cl-Br]	Presence/absence of Cl – Br at topological distance 9
4260	B09[Cl-I]	Presence/absence of Cl – I at topological distance 9
4261	B09[Cl-B]	Presence/absence of Cl – B at topological distance 9
4262	B09[Cl-Si]	Presence/absence of Cl – Si at topological distance 9
4263	B09[Cl-X]	Presence/absence of Cl – X at topological distance 9
4264	B09[Br-Br]	Presence/absence of Br – Br at topological distance 9
4265	B09[Br-I]	Presence/absence of Br – I at topological distance 9
4266	B09[Br-B]	Presence/absence of Br – B at topological distance 9
4267	B09[Br-Si]	Presence/absence of Br – Si at topological distance 9
4268	B09[Br-X]	Presence/absence of Br – X at topological distance 9
4269	B09[I-I]	Presence/absence of I – I at topological distance 9
4270	B09[I-B]	Presence/absence of I – B at topological distance 9
4271	B09[I-Si]	Presence/absence of I – Si at topological distance 9
4272	B09[I-X]	Presence/absence of I – X at topological distance 9
4273	B09[B-B]	Presence/absence of B – B at topological distance 9
4274	B09[B-Si]	Presence/absence of B – Si at topological distance 9
4275	B09[B-X]	Presence/absence of B – X at topological distance 9
4276	B09[Si-Si]	Presence/absence of Si – Si at topological distance 9
4277	B09[Si-X]	Presence/absence of Si – X at topological distance 9
4278	B09[X-X]	Presence/absence of X – X at topological distance 9
4279	B10[C-C]	Presence/absence of C – C at topological distance 10
4280	B10[C-N]	Presence/absence of C – N at topological distance 10
4281	B10[C-O]	Presence/absence of C – O at topological distance 10
4282	B10[C-S]	Presence/absence of C – S at topological distance 10
4283	B10[C-P]	Presence/absence of C – P at topological distance 10
4284	B10[C-F]	Presence/absence of C – F at topological distance 10
4285	B10[C-Cl]	Presence/absence of C – Cl at topological distance 10
4286	B10[C-Br]	Presence/absence of C – Br at topological distance 10
4287	B10[C-I]	Presence/absence of C – I at topological distance 10
4288	B10[C-B]	Presence/absence of C – B at topological distance 10
4289	B10[C-Si]	Presence/absence of C – Si at topological distance 10
4290	B10[C-X]	Presence/absence of C – X at topological distance 10
4291	B10[N-N]	Presence/absence of N – N at topological distance 10
4292	B10[N-O]	Presence/absence of N – O at topological distance 10
4293	B10[N-S]	Presence/absence of N – S at topological distance 10

4294	B10[N-P]	Presence/absence of N – P at topological distance 10
4295	B10[N-F]	Presence/absence of N – F at topological distance 10
4296	B10[N-Cl]	Presence/absence of N – Cl at topological distance 10
4297	B10[N-Br]	Presence/absence of N – Br at topological distance 10
4298	B10[N-I]	Presence/absence of N – I at topological distance 10
4299	B10[N-B]	Presence/absence of N – B at topological distance 10
4300	B10[N-Si]	Presence/absence of N – Si at topological distance 10
4301	B10[N-X]	Presence/absence of N – X at topological distance 10
4302	B10[O-O]	Presence/absence of O – O at topological distance 10
4303	B10[O-S]	Presence/absence of O – S at topological distance 10
4304	B10[O-P]	Presence/absence of O – P at topological distance 10
4305	B10[O-F]	Presence/absence of O – F at topological distance 10
4306	B10[O-Cl]	Presence/absence of O – Cl at topological distance 10
4307	B10[O-Br]	Presence/absence of O – Br at topological distance 10
4308	B10[O-I]	Presence/absence of O – I at topological distance 10
4309	B10[O-B]	Presence/absence of O – B at topological distance 10
4310	B10[O-Si]	Presence/absence of O – Si at topological distance 10
4311	B10[O-X]	Presence/absence of O – X at topological distance 10
4312	B10[S-S]	Presence/absence of S – S at topological distance 10
4313	B10[S-P]	Presence/absence of S – P at topological distance 10
4314	B10[S-F]	Presence/absence of S – F at topological distance 10
4315	B10[S-Cl]	Presence/absence of S – Cl at topological distance 10
4316	B10[S-Br]	Presence/absence of S – Br at topological distance 10
4317	B10[S-I]	Presence/absence of S – I at topological distance 10
4318	B10[S-B]	Presence/absence of S – B at topological distance 10
4319	B10[S-Si]	Presence/absence of S – Si at topological distance 10
4320	B10[S-X]	Presence/absence of S – X at topological distance 10
4321	B10[P-P]	Presence/absence of P – P at topological distance 10
4322	B10[P-F]	Presence/absence of P – F at topological distance 10
4323	B10[P-Cl]	Presence/absence of P – Cl at topological distance 10
4324	B10[P-Br]	Presence/absence of P – Br at topological distance 10
4325	B10[P-I]	Presence/absence of P – I at topological distance 10
4326	B10[P-B]	Presence/absence of P – B at topological distance 10
4327	B10[P-Si]	Presence/absence of P – Si at topological distance 10
4328	B10[P-X]	Presence/absence of P – X at topological distance 10
4329	B10[F-F]	Presence/absence of F – F at topological distance 10
4330	B10[F-Cl]	Presence/absence of F – Cl at topological distance 10
4331	B10[F-Br]	Presence/absence of F – Br at topological distance 10
4332	B10[F-I]	Presence/absence of F – I at topological distance 10
4333	B10[F-B]	Presence/absence of F – B at topological distance 10
4334	B10[F-Si]	Presence/absence of F – Si at topological distance 10
4335	B10[F-X]	Presence/absence of F – X at topological distance 10

4336	B10[Cl-Cl]	Presence/absence of Cl – Cl at topological distance 10
4337	B10[Cl-Br]	Presence/absence of Cl – Br at topological distance 10
4338	B10[Cl-I]	Presence/absence of Cl – I at topological distance 10
4339	B10[Cl-B]	Presence/absence of Cl – B at topological distance 10
4340	B10[Cl-Si]	Presence/absence of Cl – Si at topological distance 10
4341	B10[Cl-X]	Presence/absence of Cl – X at topological distance 10
4342	B10[Br-Br]	Presence/absence of Br – Br at topological distance 10
4343	B10[Br-I]	Presence/absence of Br – I at topological distance 10
4344	B10[Br-B]	Presence/absence of Br – B at topological distance 10
4345	B10[Br-Si]	Presence/absence of Br – Si at topological distance 10
4346	B10[Br-X]	Presence/absence of Br – X at topological distance 10
4347	B10[I-I]	Presence/absence of I – I at topological distance 10
4348	B10[I-B]	Presence/absence of I – B at topological distance 10
4349	B10[I-Si]	Presence/absence of I – Si at topological distance 10
4350	B10[I-X]	Presence/absence of I – X at topological distance 10
4351	B10[B-B]	Presence/absence of B – B at topological distance 10
4352	B10[B-Si]	Presence/absence of B – Si at topological distance 10
4353	B10[B-X]	Presence/absence of B – X at topological distance 10
4354	B10[Si-Si]	Presence/absence of Si – Si at topological distance 10
4355	B10[Si-X]	Presence/absence of Si – X at topological distance 10
4356	B10[X-X]	Presence/absence of X – X at topological distance 10
4357	F01[C-C]	Frequency of C – C at topological distance 1
4358	F01[C-N]	Frequency of C – N at topological distance 1
4359	F01[C-O]	Frequency of C – O at topological distance 1
4360	F01[C-S]	Frequency of C – S at topological distance 1
4361	F01[C-P]	Frequency of C – P at topological distance 1
4362	F01[C-F]	Frequency of C – F at topological distance 1
4363	F01[C-Cl]	Frequency of C – Cl at topological distance 1
4364	F01[C-Br]	Frequency of C – Br at topological distance 1
4365	F01[C-I]	Frequency of C – I at topological distance 1
4366	F01[C-B]	Frequency of C – B at topological distance 1
4367	F01[C-Si]	Frequency of C – Si at topological distance 1
4368	F01[C-X]	Frequency of C – X at topological distance 1
4369	F01[N-N]	Frequency of N – N at topological distance 1
4370	F01[N-O]	Frequency of N – O at topological distance 1
4371	F01[N-S]	Frequency of N – S at topological distance 1
4372	F01[N-P]	Frequency of N – P at topological distance 1
4373	F01[N-F]	Frequency of N – F at topological distance 1
4374	F01[N-Cl]	Frequency of N – Cl at topological distance 1
4375	F01[N-Br]	Frequency of N – Br at topological distance 1
4376	F01[N-I]	Frequency of N – I at topological distance 1
4377	F01[N-B]	Frequency of N – B at topological distance 1

4378	F01[N-Si]	Frequency of N – Si at topological distance 1
4379	F01[N-X]	Frequency of N – X at topological distance 1
4380	F01[O-O]	Frequency of O – O at topological distance 1
4381	F01[O-S]	Frequency of O – S at topological distance 1
4382	F01[O-P]	Frequency of O – P at topological distance 1
4383	F01[O-F]	Frequency of O – F at topological distance 1
4384	F01[O-Cl]	Frequency of O – Cl at topological distance 1
4385	F01[O-Br]	Frequency of O – Br at topological distance 1
4386	F01[O-I]	Frequency of O – I at topological distance 1
4387	F01[O-B]	Frequency of O – B at topological distance 1
4388	F01[O-Si]	Frequency of O – Si at topological distance 1
4389	F01[O-X]	Frequency of O – X at topological distance 1
4390	F01[S-S]	Frequency of S – S at topological distance 1
4391	F01[S-P]	Frequency of S – P at topological distance 1
4392	F01[S-F]	Frequency of S – F at topological distance 1
4393	F01[S-Cl]	Frequency of S – Cl at topological distance 1
4394	F01[S-Br]	Frequency of S – Br at topological distance 1
4395	F01[S-I]	Frequency of S – I at topological distance 1
4396	F01[S-B]	Frequency of S – B at topological distance 1
4397	F01[S-Si]	Frequency of S – Si at topological distance 1
4398	F01[S-X]	Frequency of S – X at topological distance 1
4399	F01[P-P]	Frequency of P – P at topological distance 1
4400	F01[P-F]	Frequency of P – F at topological distance 1
4401	F01[P-Cl]	Frequency of P – Cl at topological distance 1
4402	F01[P-Br]	Frequency of P – Br at topological distance 1
4403	F01[P-I]	Frequency of P – I at topological distance 1
4404	F01[P-B]	Frequency of P – B at topological distance 1
4405	F01[P-Si]	Frequency of P – Si at topological distance 1
4406	F01[P-X]	Frequency of P – X at topological distance 1
4407	F01[F-F]	Frequency of F – F at topological distance 1
4408	F01[F-Cl]	Frequency of F – Cl at topological distance 1
4409	F01[F-Br]	Frequency of F – Br at topological distance 1
4410	F01[F-I]	Frequency of F – I at topological distance 1
4411	F01[F-B]	Frequency of F – B at topological distance 1
4412	F01[F-Si]	Frequency of F – Si at topological distance 1
4413	F01[F-X]	Frequency of F – X at topological distance 1
4414	F01[Cl-Cl]	Frequency of Cl – Cl at topological distance 1
4415	F01[Cl-Br]	Frequency of Cl – Br at topological distance 1
4416	F01[Cl-I]	Frequency of Cl – I at topological distance 1
4417	F01[Cl-B]	Frequency of Cl – B at topological distance 1
4418	F01[Cl-Si]	Frequency of Cl – Si at topological distance 1
4419	F01[Cl-X]	Frequency of Cl – X at topological distance 1

4420	F01[Br-Br]	Frequency of Br – Br at topological distance 1
4421	F01[Br-I]	Frequency of Br – I at topological distance 1
4422	F01[Br-B]	Frequency of Br – B at topological distance 1
4423	F01[Br-Si]	Frequency of Br – Si at topological distance 1
4424	F01[Br-X]	Frequency of Br – X at topological distance 1
4425	F01[I-I]	Frequency of I – I at topological distance 1
4426	F01[I-B]	Frequency of I – B at topological distance 1
4427	F01[I-Si]	Frequency of I – Si at topological distance 1
4428	F01[I-X]	Frequency of I – X at topological distance 1
4429	F01[B-B]	Frequency of B – B at topological distance 1
4430	F01[B-Si]	Frequency of B – Si at topological distance 1
4431	F01[B-X]	Frequency of B – X at topological distance 1
4432	F01[Si-Si]	Frequency of Si – Si at topological distance 1
4433	F01[Si-X]	Frequency of Si – X at topological distance 1
4434	F01[X-X]	Frequency of X – X at topological distance 1
4435	F02[C-C]	Frequency of C – C at topological distance 2
4436	F02[C-N]	Frequency of C – N at topological distance 2
4437	F02[C-O]	Frequency of C – O at topological distance 2
4438	F02[C-S]	Frequency of C – S at topological distance 2
4439	F02[C-P]	Frequency of C – P at topological distance 2
4440	F02[C-F]	Frequency of C – F at topological distance 2
4441	F02[C-Cl]	Frequency of C – Cl at topological distance 2
4442	F02[C-Br]	Frequency of C – Br at topological distance 2
4443	F02[C-I]	Frequency of C – I at topological distance 2
4444	F02[C-B]	Frequency of C – B at topological distance 2
4445	F02[C-Si]	Frequency of C – Si at topological distance 2
4446	F02[C-X]	Frequency of C – X at topological distance 2
4447	F02[N-N]	Frequency of N – N at topological distance 2
4448	F02[N-O]	Frequency of N – O at topological distance 2
4449	F02[N-S]	Frequency of N – S at topological distance 2
4450	F02[N-P]	Frequency of N – P at topological distance 2
4451	F02[N-F]	Frequency of N – F at topological distance 2
4452	F02[N-Cl]	Frequency of N – Cl at topological distance 2
4453	F02[N-Br]	Frequency of N – Br at topological distance 2
4454	F02[N-I]	Frequency of N – I at topological distance 2
4455	F02[N-B]	Frequency of N – B at topological distance 2
4456	F02[N-Si]	Frequency of N – Si at topological distance 2
4457	F02[N-X]	Frequency of N – X at topological distance 2
4458	F02[O-O]	Frequency of O – O at topological distance 2
4459	F02[O-S]	Frequency of O – S at topological distance 2
4460	F02[O-P]	Frequency of O – P at topological distance 2
4461	F02[O-F]	Frequency of O – F at topological distance 2

4462	F02[O-Cl]	Frequency of O – Cl at topological distance 2
4463	F02[O-Br]	Frequency of O – Br at topological distance 2
4464	F02[O-I]	Frequency of O – I at topological distance 2
4465	F02[O-B]	Frequency of O – B at topological distance 2
4466	F02[O-Si]	Frequency of O – Si at topological distance 2
4467	F02[O-X]	Frequency of O – X at topological distance 2
4468	F02[S-S]	Frequency of S – S at topological distance 2
4469	F02[S-P]	Frequency of S – P at topological distance 2
4470	F02[S-F]	Frequency of S – F at topological distance 2
4471	F02[S-Cl]	Frequency of S – Cl at topological distance 2
4472	F02[S-Br]	Frequency of S – Br at topological distance 2
4473	F02[S-I]	Frequency of S – I at topological distance 2
4474	F02[S-B]	Frequency of S – B at topological distance 2
4475	F02[S-Si]	Frequency of S – Si at topological distance 2
4476	F02[S-X]	Frequency of S – X at topological distance 2
4477	F02[P-P]	Frequency of P – P at topological distance 2
4478	F02[P-F]	Frequency of P – F at topological distance 2
4479	F02[P-Cl]	Frequency of P – Cl at topological distance 2
4480	F02[P-Br]	Frequency of P – Br at topological distance 2
4481	F02[P-I]	Frequency of P – I at topological distance 2
4482	F02[P-B]	Frequency of P – B at topological distance 2
4483	F02[P-Si]	Frequency of P – Si at topological distance 2
4484	F02[P-X]	Frequency of P – X at topological distance 2
4485	F02[F-F]	Frequency of F – F at topological distance 2
4486	F02[F-Cl]	Frequency of F – Cl at topological distance 2
4487	F02[F-Br]	Frequency of F – Br at topological distance 2
4488	F02[F-I]	Frequency of F – I at topological distance 2
4489	F02[F-B]	Frequency of F – B at topological distance 2
4490	F02[F-Si]	Frequency of F – Si at topological distance 2
4491	F02[F-X]	Frequency of F – X at topological distance 2
4492	F02[Cl-Cl]	Frequency of Cl – Cl at topological distance 2
4493	F02[Cl-Br]	Frequency of Cl – Br at topological distance 2
4494	F02[Cl-I]	Frequency of Cl – I at topological distance 2
4495	F02[Cl-B]	Frequency of Cl – B at topological distance 2
4496	F02[Cl-Si]	Frequency of Cl – Si at topological distance 2
4497	F02[Cl-X]	Frequency of Cl – X at topological distance 2
4498	F02[Br-Br]	Frequency of Br – Br at topological distance 2
4499	F02[Br-I]	Frequency of Br – I at topological distance 2
4500	F02[Br-B]	Frequency of Br – B at topological distance 2
4501	F02[Br-Si]	Frequency of Br – Si at topological distance 2
4502	F02[Br-X]	Frequency of Br – X at topological distance 2
4503	F02[I-I]	Frequency of I – I at topological distance 2

4504	F02[I-B]	Frequency of I – B at topological distance 2
4505	F02[I-Si]	Frequency of I – Si at topological distance 2
4506	F02[I-X]	Frequency of I – X at topological distance 2
4507	F02[B-B]	Frequency of B – B at topological distance 2
4508	F02[B-Si]	Frequency of B – Si at topological distance 2
4509	F02[B-X]	Frequency of B – X at topological distance 2
4510	F02[Si-Si]	Frequency of Si – Si at topological distance 2
4511	F02[Si-X]	Frequency of Si – X at topological distance 2
4512	F02[X-X]	Frequency of X – X at topological distance 2
4513	F03[C-C]	Frequency of C – C at topological distance 3
4514	F03[C-N]	Frequency of C – N at topological distance 3
4515	F03[C-O]	Frequency of C – O at topological distance 3
4516	F03[C-S]	Frequency of C – S at topological distance 3
4517	F03[C-P]	Frequency of C – P at topological distance 3
4518	F03[C-F]	Frequency of C – F at topological distance 3
4519	F03[C-Cl]	Frequency of C – Cl at topological distance 3
4520	F03[C-Br]	Frequency of C – Br at topological distance 3
4521	F03[C-I]	Frequency of C – I at topological distance 3
4522	F03[C-B]	Frequency of C – B at topological distance 3
4523	F03[C-Si]	Frequency of C – Si at topological distance 3
4524	F03[C-X]	Frequency of C – X at topological distance 3
4525	F03[N-N]	Frequency of N – N at topological distance 3
4526	F03[N-O]	Frequency of N – O at topological distance 3
4527	F03[N-S]	Frequency of N – S at topological distance 3
4528	F03[N-P]	Frequency of N – P at topological distance 3
4529	F03[N-F]	Frequency of N – F at topological distance 3
4530	F03[N-Cl]	Frequency of N – Cl at topological distance 3
4531	F03[N-Br]	Frequency of N – Br at topological distance 3
4532	F03[N-I]	Frequency of N – I at topological distance 3
4533	F03[N-B]	Frequency of N – B at topological distance 3
4534	F03[N-Si]	Frequency of N – Si at topological distance 3
4535	F03[N-X]	Frequency of N – X at topological distance 3
4536	F03[O-O]	Frequency of O – O at topological distance 3
4537	F03[O-S]	Frequency of O – S at topological distance 3
4538	F03[O-P]	Frequency of O – P at topological distance 3
4539	F03[O-F]	Frequency of O – F at topological distance 3
4540	F03[O-Cl]	Frequency of O – Cl at topological distance 3
4541	F03[O-Br]	Frequency of O – Br at topological distance 3
4542	F03[O-I]	Frequency of O – I at topological distance 3
4543	F03[O-B]	Frequency of O – B at topological distance 3
4544	F03[O-Si]	Frequency of O – Si at topological distance 3
4545	F03[O-X]	Frequency of O – X at topological distance 3

4546	F03[S-S]	Frequency of S – S at topological distance 3
4547	F03[S-P]	Frequency of S – P at topological distance 3
4548	F03[S-F]	Frequency of S – F at topological distance 3
4549	F03[S-Cl]	Frequency of S – Cl at topological distance 3
4550	F03[S-Br]	Frequency of S – Br at topological distance 3
4551	F03[S-I]	Frequency of S – I at topological distance 3
4552	F03[S-B]	Frequency of S – B at topological distance 3
4553	F03[S-Si]	Frequency of S – Si at topological distance 3
4554	F03[S-X]	Frequency of S – X at topological distance 3
4555	F03[P-P]	Frequency of P – P at topological distance 3
4556	F03[P-F]	Frequency of P – F at topological distance 3
4557	F03[P-Cl]	Frequency of P – Cl at topological distance 3
4558	F03[P-Br]	Frequency of P – Br at topological distance 3
4559	F03[P-I]	Frequency of P – I at topological distance 3
4560	F03[P-B]	Frequency of P – B at topological distance 3
4561	F03[P-Si]	Frequency of P – Si at topological distance 3
4562	F03[P-X]	Frequency of P – X at topological distance 3
4563	F03[F-F]	Frequency of F – F at topological distance 3
4564	F03[F-Cl]	Frequency of F – Cl at topological distance 3
4565	F03[F-Br]	Frequency of F – Br at topological distance 3
4566	F03[F-I]	Frequency of F – I at topological distance 3
4567	F03[F-B]	Frequency of F – B at topological distance 3
4568	F03[F-Si]	Frequency of F – Si at topological distance 3
4569	F03[F-X]	Frequency of F – X at topological distance 3
4570	F03[Cl-Cl]	Frequency of Cl – Cl at topological distance 3
4571	F03[Cl-Br]	Frequency of Cl – Br at topological distance 3
4572	F03[Cl-I]	Frequency of Cl – I at topological distance 3
4573	F03[Cl-B]	Frequency of Cl – B at topological distance 3
4574	F03[Cl-Si]	Frequency of Cl – Si at topological distance 3
4575	F03[Cl-X]	Frequency of Cl – X at topological distance 3
4576	F03[Br-Br]	Frequency of Br – Br at topological distance 3
4577	F03[Br-I]	Frequency of Br – I at topological distance 3
4578	F03[Br-B]	Frequency of Br – B at topological distance 3
4579	F03[Br-Si]	Frequency of Br – Si at topological distance 3
4580	F03[Br-X]	Frequency of Br – X at topological distance 3
4581	F03[I-I]	Frequency of I – I at topological distance 3
4582	F03[I-B]	Frequency of I – B at topological distance 3
4583	F03[I-Si]	Frequency of I – Si at topological distance 3
4584	F03[I-X]	Frequency of I – X at topological distance 3
4585	F03[B-B]	Frequency of B – B at topological distance 3
4586	F03[B-Si]	Frequency of B – Si at topological distance 3
4587	F03[B-X]	Frequency of B – X at topological distance 3

4588	F03[Si-Si]	Frequency of Si – Si at topological distance 3
4589	F03[Si-X]	Frequency of Si – X at topological distance 3
4590	F03[X-X]	Frequency of X – X at topological distance 3
4591	F04[C-C]	Frequency of C – C at topological distance 4
4592	F04[C-N]	Frequency of C – N at topological distance 4
4593	F04[C-O]	Frequency of C – O at topological distance 4
4594	F04[C-S]	Frequency of C – S at topological distance 4
4595	F04[C-P]	Frequency of C – P at topological distance 4
4596	F04[C-F]	Frequency of C – F at topological distance 4
4597	F04[C-Cl]	Frequency of C – Cl at topological distance 4
4598	F04[C-Br]	Frequency of C – Br at topological distance 4
4599	F04[C-I]	Frequency of C – I at topological distance 4
4600	F04[C-B]	Frequency of C – B at topological distance 4
4601	F04[C-Si]	Frequency of C – Si at topological distance 4
4602	F04[C-X]	Frequency of C – X at topological distance 4
4603	F04[N-N]	Frequency of N – N at topological distance 4
4604	F04[N-O]	Frequency of N – O at topological distance 4
4605	F04[N-S]	Frequency of N – S at topological distance 4
4606	F04[N-P]	Frequency of N – P at topological distance 4
4607	F04[N-F]	Frequency of N – F at topological distance 4
4608	F04[N-Cl]	Frequency of N – Cl at topological distance 4
4609	F04[N-Br]	Frequency of N – Br at topological distance 4
4610	F04[N-I]	Frequency of N – I at topological distance 4
4611	F04[N-B]	Frequency of N – B at topological distance 4
4612	F04[N-Si]	Frequency of N – Si at topological distance 4
4613	F04[N-X]	Frequency of N – X at topological distance 4
4614	F04[O-O]	Frequency of O – O at topological distance 4
4615	F04[O-S]	Frequency of O – S at topological distance 4
4616	F04[O-P]	Frequency of O – P at topological distance 4
4617	F04[O-F]	Frequency of O – F at topological distance 4
4618	F04[O-Cl]	Frequency of O – Cl at topological distance 4
4619	F04[O-Br]	Frequency of O – Br at topological distance 4
4620	F04[O-I]	Frequency of O – I at topological distance 4
4621	F04[O-B]	Frequency of O – B at topological distance 4
4622	F04[O-Si]	Frequency of O – Si at topological distance 4
4623	F04[O-X]	Frequency of O – X at topological distance 4
4624	F04[S-S]	Frequency of S – S at topological distance 4
4625	F04[S-P]	Frequency of S – P at topological distance 4
4626	F04[S-F]	Frequency of S – F at topological distance 4
4627	F04[S-Cl]	Frequency of S – Cl at topological distance 4
4628	F04[S-Br]	Frequency of S – Br at topological distance 4
4629	F04[S-I]	Frequency of S – I at topological distance 4

4630	F04[S-B]	Frequency of S – B at topological distance 4
4631	F04[S-Si]	Frequency of S – Si at topological distance 4
4632	F04[S-X]	Frequency of S – X at topological distance 4
4633	F04[P-P]	Frequency of P – P at topological distance 4
4634	F04[P-F]	Frequency of P – F at topological distance 4
4635	F04[P-Cl]	Frequency of P – Cl at topological distance 4
4636	F04[P-Br]	Frequency of P – Br at topological distance 4
4637	F04[P-I]	Frequency of P – I at topological distance 4
4638	F04[P-B]	Frequency of P – B at topological distance 4
4639	F04[P-Si]	Frequency of P – Si at topological distance 4
4640	F04[P-X]	Frequency of P – X at topological distance 4
4641	F04[F-F]	Frequency of F – F at topological distance 4
4642	F04[F-Cl]	Frequency of F – Cl at topological distance 4
4643	F04[F-Br]	Frequency of F – Br at topological distance 4
4644	F04[F-I]	Frequency of F – I at topological distance 4
4645	F04[F-B]	Frequency of F – B at topological distance 4
4646	F04[F-Si]	Frequency of F – Si at topological distance 4
4647	F04[F-X]	Frequency of F – X at topological distance 4
4648	F04[Cl-Cl]	Frequency of Cl – Cl at topological distance 4
4649	F04[Cl-Br]	Frequency of Cl – Br at topological distance 4
4650	F04[Cl-I]	Frequency of Cl – I at topological distance 4
4651	F04[Cl-B]	Frequency of Cl – B at topological distance 4
4652	F04[Cl-Si]	Frequency of Cl – Si at topological distance 4
4653	F04[Cl-X]	Frequency of Cl – X at topological distance 4
4654	F04[Br-Br]	Frequency of Br – Br at topological distance 4
4655	F04[Br-I]	Frequency of Br – I at topological distance 4
4656	F04[Br-B]	Frequency of Br – B at topological distance 4
4657	F04[Br-Si]	Frequency of Br – Si at topological distance 4
4658	F04[Br-X]	Frequency of Br – X at topological distance 4
4659	F04[I-I]	Frequency of I – I at topological distance 4
4660	F04[I-B]	Frequency of I – B at topological distance 4
4661	F04[I-Si]	Frequency of I – Si at topological distance 4
4662	F04[I-X]	Frequency of I – X at topological distance 4
4663	F04[B-B]	Frequency of B – B at topological distance 4
4664	F04[B-Si]	Frequency of B – Si at topological distance 4
4665	F04[B-X]	Frequency of B – X at topological distance 4
4666	F04[Si-Si]	Frequency of Si – Si at topological distance 4
4667	F04[Si-X]	Frequency of Si – X at topological distance 4
4668	F04[X-X]	Frequency of X – X at topological distance 4
4669	F05[C-C]	Frequency of C – C at topological distance 5
4670	F05[C-N]	Frequency of C – N at topological distance 5
4671	F05[C-O]	Frequency of C – O at topological distance 5

4672	F05[C-S]	Frequency of C – S at topological distance 5
4673	F05[C-P]	Frequency of C – P at topological distance 5
4674	F05[C-F]	Frequency of C – F at topological distance 5
4675	F05[C-Cl]	Frequency of C – Cl at topological distance 5
4676	F05[C-Br]	Frequency of C – Br at topological distance 5
4677	F05[C-I]	Frequency of C – I at topological distance 5
4678	F05[C-B]	Frequency of C – B at topological distance 5
4679	F05[C-Si]	Frequency of C – Si at topological distance 5
4680	F05[C-X]	Frequency of C – X at topological distance 5
4681	F05[N-N]	Frequency of N – N at topological distance 5
4682	F05[N-O]	Frequency of N – O at topological distance 5
4683	F05[N-S]	Frequency of N – S at topological distance 5
4684	F05[N-P]	Frequency of N – P at topological distance 5
4685	F05[N-F]	Frequency of N – F at topological distance 5
4686	F05[N-Cl]	Frequency of N – Cl at topological distance 5
4687	F05[N-Br]	Frequency of N – Br at topological distance 5
4688	F05[N-I]	Frequency of N – I at topological distance 5
4689	F05[N-B]	Frequency of N – B at topological distance 5
4690	F05[N-Si]	Frequency of N – Si at topological distance 5
4691	F05[N-X]	Frequency of N – X at topological distance 5
4692	F05[O-O]	Frequency of O – O at topological distance 5
4693	F05[O-S]	Frequency of O – S at topological distance 5
4694	F05[O-P]	Frequency of O – P at topological distance 5
4695	F05[O-F]	Frequency of O – F at topological distance 5
4696	F05[O-Cl]	Frequency of O – Cl at topological distance 5
4697	F05[O-Br]	Frequency of O – Br at topological distance 5
4698	F05[O-I]	Frequency of O – I at topological distance 5
4699	F05[O-B]	Frequency of O – B at topological distance 5
4700	F05[O-Si]	Frequency of O – Si at topological distance 5
4701	F05[O-X]	Frequency of O – X at topological distance 5
4702	F05[S-S]	Frequency of S – S at topological distance 5
4703	F05[S-P]	Frequency of S – P at topological distance 5
4704	F05[S-F]	Frequency of S – F at topological distance 5
4705	F05[S-Cl]	Frequency of S – Cl at topological distance 5
4706	F05[S-Br]	Frequency of S – Br at topological distance 5
4707	F05[S-I]	Frequency of S – I at topological distance 5
4708	F05[S-B]	Frequency of S – B at topological distance 5
4709	F05[S-Si]	Frequency of S – Si at topological distance 5
4710	F05[S-X]	Frequency of S – X at topological distance 5
4711	F05[P-P]	Frequency of P – P at topological distance 5
4712	F05[P-F]	Frequency of P – F at topological distance 5
4713	F05[P-Cl]	Frequency of P – Cl at topological distance 5

4714	F05[P-Br]	Frequency of P – Br at topological distance 5
4715	F05[P-I]	Frequency of P – I at topological distance 5
4716	F05[P-B]	Frequency of P – B at topological distance 5
4717	F05[P-Si]	Frequency of P – Si at topological distance 5
4718	F05[P-X]	Frequency of P – X at topological distance 5
4719	F05[F-F]	Frequency of F – F at topological distance 5
4720	F05[F-Cl]	Frequency of F – Cl at topological distance 5
4721	F05[F-Br]	Frequency of F – Br at topological distance 5
4722	F05[F-I]	Frequency of F – I at topological distance 5
4723	F05[F-B]	Frequency of F – B at topological distance 5
4724	F05[F-Si]	Frequency of F – Si at topological distance 5
4725	F05[F-X]	Frequency of F – X at topological distance 5
4726	F05[Cl-Cl]	Frequency of Cl – Cl at topological distance 5
4727	F05[Cl-Br]	Frequency of Cl – Br at topological distance 5
4728	F05[Cl-I]	Frequency of Cl – I at topological distance 5
4729	F05[Cl-B]	Frequency of Cl – B at topological distance 5
4730	F05[Cl-Si]	Frequency of Cl – Si at topological distance 5
4731	F05[Cl-X]	Frequency of Cl – X at topological distance 5
4732	F05[Br-Br]	Frequency of Br – Br at topological distance 5
4733	F05[Br-I]	Frequency of Br – I at topological distance 5
4734	F05[Br-B]	Frequency of Br – B at topological distance 5
4735	F05[Br-Si]	Frequency of Br – Si at topological distance 5
4736	F05[Br-X]	Frequency of Br – X at topological distance 5
4737	F05[I-I]	Frequency of I – I at topological distance 5
4738	F05[I-B]	Frequency of I – B at topological distance 5
4739	F05[I-Si]	Frequency of I – Si at topological distance 5
4740	F05[I-X]	Frequency of I – X at topological distance 5
4741	F05[B-B]	Frequency of B – B at topological distance 5
4742	F05[B-Si]	Frequency of B – Si at topological distance 5
4743	F05[B-X]	Frequency of B – X at topological distance 5
4744	F05[Si-Si]	Frequency of Si – Si at topological distance 5
4745	F05[Si-X]	Frequency of Si – X at topological distance 5
4746	F05[X-X]	Frequency of X – X at topological distance 5
4747	F06[C-C]	Frequency of C – C at topological distance 6
4748	F06[C-N]	Frequency of C – N at topological distance 6
4749	F06[C-O]	Frequency of C – O at topological distance 6
4750	F06[C-S]	Frequency of C – S at topological distance 6
4751	F06[C-P]	Frequency of C – P at topological distance 6
4752	F06[C-F]	Frequency of C – F at topological distance 6
4753	F06[C-Cl]	Frequency of C – Cl at topological distance 6
4754	F06[C-Br]	Frequency of C – Br at topological distance 6
4755	F06[C-I]	Frequency of C – I at topological distance 6

4756	F06[C-B]	Frequency of C – B at topological distance 6
4757	F06[C-Si]	Frequency of C – Si at topological distance 6
4758	F06[C-X]	Frequency of C – X at topological distance 6
4759	F06[N-N]	Frequency of N – N at topological distance 6
4760	F06[N-O]	Frequency of N – O at topological distance 6
4761	F06[N-S]	Frequency of N – S at topological distance 6
4762	F06[N-P]	Frequency of N – P at topological distance 6
4763	F06[N-F]	Frequency of N – F at topological distance 6
4764	F06[N-Cl]	Frequency of N – Cl at topological distance 6
4765	F06[N-Br]	Frequency of N – Br at topological distance 6
4766	F06[N-I]	Frequency of N – I at topological distance 6
4767	F06[N-B]	Frequency of N – B at topological distance 6
4768	F06[N-Si]	Frequency of N – Si at topological distance 6
4769	F06[N-X]	Frequency of N – X at topological distance 6
4770	F06[O-O]	Frequency of O – O at topological distance 6
4771	F06[O-S]	Frequency of O – S at topological distance 6
4772	F06[O-P]	Frequency of O – P at topological distance 6
4773	F06[O-F]	Frequency of O – F at topological distance 6
4774	F06[O-Cl]	Frequency of O – Cl at topological distance 6
4775	F06[O-Br]	Frequency of O – Br at topological distance 6
4776	F06[O-I]	Frequency of O – I at topological distance 6
4777	F06[O-B]	Frequency of O – B at topological distance 6
4778	F06[O-Si]	Frequency of O – Si at topological distance 6
4779	F06[O-X]	Frequency of O – X at topological distance 6
4780	F06[S-S]	Frequency of S – S at topological distance 6
4781	F06[S-P]	Frequency of S – P at topological distance 6
4782	F06[S-F]	Frequency of S – F at topological distance 6
4783	F06[S-Cl]	Frequency of S – Cl at topological distance 6
4784	F06[S-Br]	Frequency of S – Br at topological distance 6
4785	F06[S-I]	Frequency of S – I at topological distance 6
4786	F06[S-B]	Frequency of S – B at topological distance 6
4787	F06[S-Si]	Frequency of S – Si at topological distance 6
4788	F06[S-X]	Frequency of S – X at topological distance 6
4789	F06[P-P]	Frequency of P – P at topological distance 6
4790	F06[P-F]	Frequency of P – F at topological distance 6
4791	F06[P-Cl]	Frequency of P – Cl at topological distance 6
4792	F06[P-Br]	Frequency of P – Br at topological distance 6
4793	F06[P-I]	Frequency of P – I at topological distance 6
4794	F06[P-B]	Frequency of P – B at topological distance 6
4795	F06[P-Si]	Frequency of P – Si at topological distance 6
4796	F06[P-X]	Frequency of P – X at topological distance 6
4797	F06[F-F]	Frequency of F – F at topological distance 6

4798	F06[F-Cl]	Frequency of F – Cl at topological distance 6
4799	F06[F-Br]	Frequency of F – Br at topological distance 6
4800	F06[F-I]	Frequency of F – I at topological distance 6
4801	F06[F-B]	Frequency of F – B at topological distance 6
4802	F06[F-Si]	Frequency of F – Si at topological distance 6
4803	F06[F-X]	Frequency of F – X at topological distance 6
4804	F06[Cl-Cl]	Frequency of Cl – Cl at topological distance 6
4805	F06[Cl-Br]	Frequency of Cl – Br at topological distance 6
4806	F06[Cl-I]	Frequency of Cl – I at topological distance 6
4807	F06[Cl-B]	Frequency of Cl – B at topological distance 6
4808	F06[Cl-Si]	Frequency of Cl – Si at topological distance 6
4809	F06[Cl-X]	Frequency of Cl – X at topological distance 6
4810	F06[Br-Br]	Frequency of Br – Br at topological distance 6
4811	F06[Br-I]	Frequency of Br – I at topological distance 6
4812	F06[Br-B]	Frequency of Br – B at topological distance 6
4813	F06[Br-Si]	Frequency of Br – Si at topological distance 6
4814	F06[Br-X]	Frequency of Br – X at topological distance 6
4815	F06[I-I]	Frequency of I – I at topological distance 6
4816	F06[I-B]	Frequency of I – B at topological distance 6
4817	F06[I-Si]	Frequency of I – Si at topological distance 6
4818	F06[I-X]	Frequency of I – X at topological distance 6
4819	F06[B-B]	Frequency of B – B at topological distance 6
4820	F06[B-Si]	Frequency of B – Si at topological distance 6
4821	F06[B-X]	Frequency of B – X at topological distance 6
4822	F06[Si-Si]	Frequency of Si – Si at topological distance 6
4823	F06[Si-X]	Frequency of Si – X at topological distance 6
4824	F06[X-X]	Frequency of X – X at topological distance 6
4825	F07[C-C]	Frequency of C – C at topological distance 7
4826	F07[C-N]	Frequency of C – N at topological distance 7
4827	F07[C-O]	Frequency of C – O at topological distance 7
4828	F07[C-S]	Frequency of C – S at topological distance 7
4829	F07[C-P]	Frequency of C – P at topological distance 7
4830	F07[C-F]	Frequency of C – F at topological distance 7
4831	F07[C-Cl]	Frequency of C – Cl at topological distance 7
4832	F07[C-Br]	Frequency of C – Br at topological distance 7
4833	F07[C-I]	Frequency of C – I at topological distance 7
4834	F07[C-B]	Frequency of C – B at topological distance 7
4835	F07[C-Si]	Frequency of C – Si at topological distance 7
4836	F07[C-X]	Frequency of C – X at topological distance 7
4837	F07[N-N]	Frequency of N – N at topological distance 7
4838	F07[N-O]	Frequency of N – O at topological distance 7
4839	F07[N-S]	Frequency of N – S at topological distance 7

4840	F07[N-P]	Frequency of N – P at topological distance 7
4841	F07[N-F]	Frequency of N – F at topological distance 7
4842	F07[N-Cl]	Frequency of N – Cl at topological distance 7
4843	F07[N-Br]	Frequency of N – Br at topological distance 7
4844	F07[N-I]	Frequency of N – I at topological distance 7
4845	F07[N-B]	Frequency of N – B at topological distance 7
4846	F07[N-Si]	Frequency of N – Si at topological distance 7
4847	F07[N-X]	Frequency of N – X at topological distance 7
4848	F07[O-O]	Frequency of O – O at topological distance 7
4849	F07[O-S]	Frequency of O – S at topological distance 7
4850	F07[O-P]	Frequency of O – P at topological distance 7
4851	F07[O-F]	Frequency of O – F at topological distance 7
4852	F07[O-Cl]	Frequency of O – Cl at topological distance 7
4853	F07[O-Br]	Frequency of O – Br at topological distance 7
4854	F07[O-I]	Frequency of O – I at topological distance 7
4855	F07[O-B]	Frequency of O – B at topological distance 7
4856	F07[O-Si]	Frequency of O – Si at topological distance 7
4857	F07[O-X]	Frequency of O – X at topological distance 7
4858	F07[S-S]	Frequency of S – S at topological distance 7
4859	F07[S-P]	Frequency of S – P at topological distance 7
4860	F07[S-F]	Frequency of S – F at topological distance 7
4861	F07[S-Cl]	Frequency of S – Cl at topological distance 7
4862	F07[S-Br]	Frequency of S – Br at topological distance 7
4863	F07[S-I]	Frequency of S – I at topological distance 7
4864	F07[S-B]	Frequency of S – B at topological distance 7
4865	F07[S-Si]	Frequency of S – Si at topological distance 7
4866	F07[S-X]	Frequency of S – X at topological distance 7
4867	F07[P-P]	Frequency of P – P at topological distance 7
4868	F07[P-F]	Frequency of P – F at topological distance 7
4869	F07[P-Cl]	Frequency of P – Cl at topological distance 7
4870	F07[P-Br]	Frequency of P – Br at topological distance 7
4871	F07[P-I]	Frequency of P – I at topological distance 7
4872	F07[P-B]	Frequency of P – B at topological distance 7
4873	F07[P-Si]	Frequency of P – Si at topological distance 7
4874	F07[P-X]	Frequency of P – X at topological distance 7
4875	F07[F-F]	Frequency of F – F at topological distance 7
4876	F07[F-Cl]	Frequency of F – Cl at topological distance 7
4877	F07[F-Br]	Frequency of F – Br at topological distance 7
4878	F07[F-I]	Frequency of F – I at topological distance 7
4879	F07[F-B]	Frequency of F – B at topological distance 7
4880	F07[F-Si]	Frequency of F – Si at topological distance 7
4881	F07[F-X]	Frequency of F – X at topological distance 7

4882	F07[Cl-Cl]	Frequency of Cl – Cl at topological distance 7
4883	F07[Cl-Br]	Frequency of Cl – Br at topological distance 7
4884	F07[Cl-I]	Frequency of Cl – I at topological distance 7
4885	F07[Cl-B]	Frequency of Cl – B at topological distance 7
4886	F07[Cl-Si]	Frequency of Cl – Si at topological distance 7
4887	F07[Cl-X]	Frequency of Cl – X at topological distance 7
4888	F07[Br-Br]	Frequency of Br – Br at topological distance 7
4889	F07[Br-I]	Frequency of Br – I at topological distance 7
4890	F07[Br-B]	Frequency of Br – B at topological distance 7
4891	F07[Br-Si]	Frequency of Br – Si at topological distance 7
4892	F07[Br-X]	Frequency of Br – X at topological distance 7
4893	F07[I-I]	Frequency of I – I at topological distance 7
4894	F07[I-B]	Frequency of I – B at topological distance 7
4895	F07[I-Si]	Frequency of I – Si at topological distance 7
4896	F07[I-X]	Frequency of I – X at topological distance 7
4897	F07[B-B]	Frequency of B – B at topological distance 7
4898	F07[B-Si]	Frequency of B – Si at topological distance 7
4899	F07[B-X]	Frequency of B – X at topological distance 7
4900	F07[Si-Si]	Frequency of Si – Si at topological distance 7
4901	F07[Si-X]	Frequency of Si – X at topological distance 7
4902	F07[X-X]	Frequency of X – X at topological distance 7
4903	F08[C-C]	Frequency of C – C at topological distance 8
4904	F08[C-N]	Frequency of C – N at topological distance 8
4905	F08[C-O]	Frequency of C – O at topological distance 8
4906	F08[C-S]	Frequency of C – S at topological distance 8
4907	F08[C-P]	Frequency of C – P at topological distance 8
4908	F08[C-F]	Frequency of C – F at topological distance 8
4909	F08[C-Cl]	Frequency of C – Cl at topological distance 8
4910	F08[C-Br]	Frequency of C – Br at topological distance 8
4911	F08[C-I]	Frequency of C – I at topological distance 8
4912	F08[C-B]	Frequency of C – B at topological distance 8
4913	F08[C-Si]	Frequency of C – Si at topological distance 8
4914	F08[C-X]	Frequency of C – X at topological distance 8
4915	F08[N-N]	Frequency of N – N at topological distance 8
4916	F08[N-O]	Frequency of N – O at topological distance 8
4917	F08[N-S]	Frequency of N – S at topological distance 8
4918	F08[N-P]	Frequency of N – P at topological distance 8
4919	F08[N-F]	Frequency of N – F at topological distance 8
4920	F08[N-Cl]	Frequency of N – Cl at topological distance 8
4921	F08[N-Br]	Frequency of N – Br at topological distance 8
4922	F08[N-I]	Frequency of N – I at topological distance 8
4923	F08[N-B]	Frequency of N – B at topological distance 8

4924	F08[N-Si]	Frequency of N – Si at topological distance 8
4925	F08[N-X]	Frequency of N – X at topological distance 8
4926	F08[O-O]	Frequency of O – O at topological distance 8
4927	F08[O-S]	Frequency of O – S at topological distance 8
4928	F08[O-P]	Frequency of O – P at topological distance 8
4929	F08[O-F]	Frequency of O – F at topological distance 8
4930	F08[O-Cl]	Frequency of O – Cl at topological distance 8
4931	F08[O-Br]	Frequency of O – Br at topological distance 8
4932	F08[O-I]	Frequency of O – I at topological distance 8
4933	F08[O-B]	Frequency of O – B at topological distance 8
4934	F08[O-Si]	Frequency of O – Si at topological distance 8
4935	F08[O-X]	Frequency of O – X at topological distance 8
4936	F08[S-S]	Frequency of S – S at topological distance 8
4937	F08[S-P]	Frequency of S – P at topological distance 8
4938	F08[S-F]	Frequency of S – F at topological distance 8
4939	F08[S-Cl]	Frequency of S – Cl at topological distance 8
4940	F08[S-Br]	Frequency of S – Br at topological distance 8
4941	F08[S-I]	Frequency of S – I at topological distance 8
4942	F08[S-B]	Frequency of S – B at topological distance 8
4943	F08[S-Si]	Frequency of S – Si at topological distance 8
4944	F08[S-X]	Frequency of S – X at topological distance 8
4945	F08[P-P]	Frequency of P – P at topological distance 8
4946	F08[P-F]	Frequency of P – F at topological distance 8
4947	F08[P-Cl]	Frequency of P – Cl at topological distance 8
4948	F08[P-Br]	Frequency of P – Br at topological distance 8
4949	F08[P-I]	Frequency of P – I at topological distance 8
4950	F08[P-B]	Frequency of P – B at topological distance 8
4951	F08[P-Si]	Frequency of P – Si at topological distance 8
4952	F08[P-X]	Frequency of P – X at topological distance 8
4953	F08[F-F]	Frequency of F – F at topological distance 8
4954	F08[F-Cl]	Frequency of F – Cl at topological distance 8
4955	F08[F-Br]	Frequency of F – Br at topological distance 8
4956	F08[F-I]	Frequency of F – I at topological distance 8
4957	F08[F-B]	Frequency of F – B at topological distance 8
4958	F08[F-Si]	Frequency of F – Si at topological distance 8
4959	F08[F-X]	Frequency of F – X at topological distance 8
4960	F08[Cl-Cl]	Frequency of Cl – Cl at topological distance 8
4961	F08[Cl-Br]	Frequency of Cl – Br at topological distance 8
4962	F08[Cl-I]	Frequency of Cl – I at topological distance 8
4963	F08[Cl-B]	Frequency of Cl – B at topological distance 8
4964	F08[Cl-Si]	Frequency of Cl – Si at topological distance 8
4965	F08[Cl-X]	Frequency of Cl – X at topological distance 8

4966	F08[Br-Br]	Frequency of Br – Br at topological distance 8
4967	F08[Br-I]	Frequency of Br – I at topological distance 8
4968	F08[Br-B]	Frequency of Br – B at topological distance 8
4969	F08[Br-Si]	Frequency of Br – Si at topological distance 8
4970	F08[Br-X]	Frequency of Br – X at topological distance 8
4971	F08[I-I]	Frequency of I – I at topological distance 8
4972	F08[I-B]	Frequency of I – B at topological distance 8
4973	F08[I-Si]	Frequency of I – Si at topological distance 8
4974	F08[I-X]	Frequency of I – X at topological distance 8
4975	F08[B-B]	Frequency of B – B at topological distance 8
4976	F08[B-Si]	Frequency of B – Si at topological distance 8
4977	F08[B-X]	Frequency of B – X at topological distance 8
4978	F08[Si-Si]	Frequency of Si – Si at topological distance 8
4979	F08[Si-X]	Frequency of Si – X at topological distance 8
4980	F08[X-X]	Frequency of X – X at topological distance 8
4981	F09[C-C]	Frequency of C – C at topological distance 9
4982	F09[C-N]	Frequency of C – N at topological distance 9
4983	F09[C-O]	Frequency of C – O at topological distance 9
4984	F09[C-S]	Frequency of C – S at topological distance 9
4985	F09[C-P]	Frequency of C – P at topological distance 9
4986	F09[C-F]	Frequency of C – F at topological distance 9
4987	F09[C-Cl]	Frequency of C – Cl at topological distance 9
4988	F09[C-Br]	Frequency of C – Br at topological distance 9
4989	F09[C-I]	Frequency of C – I at topological distance 9
4990	F09[C-B]	Frequency of C – B at topological distance 9
4991	F09[C-Si]	Frequency of C – Si at topological distance 9
4992	F09[C-X]	Frequency of C – X at topological distance 9
4993	F09[N-N]	Frequency of N – N at topological distance 9
4994	F09[N-O]	Frequency of N – O at topological distance 9
4995	F09[N-S]	Frequency of N – S at topological distance 9
4996	F09[N-P]	Frequency of N – P at topological distance 9
4997	F09[N-F]	Frequency of N – F at topological distance 9
4998	F09[N-Cl]	Frequency of N – Cl at topological distance 9
4999	F09[N-Br]	Frequency of N – Br at topological distance 9
5000	F09[N-I]	Frequency of N – I at topological distance 9
5001	F09[N-B]	Frequency of N – B at topological distance 9
5002	F09[N-Si]	Frequency of N – Si at topological distance 9
5003	F09[N-X]	Frequency of N – X at topological distance 9
5004	F09[O-O]	Frequency of O – O at topological distance 9
5005	F09[O-S]	Frequency of O – S at topological distance 9
5006	F09[O-P]	Frequency of O – P at topological distance 9
5007	F09[O-F]	Frequency of O – F at topological distance 9

5008	F09[O-Cl]	Frequency of O – Cl at topological distance 9
5009	F09[O-Br]	Frequency of O – Br at topological distance 9
5010	F09[O-I]	Frequency of O – I at topological distance 9
5011	F09[O-B]	Frequency of O – B at topological distance 9
5012	F09[O-Si]	Frequency of O – Si at topological distance 9
5013	F09[O-X]	Frequency of O – X at topological distance 9
5014	F09[S-S]	Frequency of S – S at topological distance 9
5015	F09[S-P]	Frequency of S – P at topological distance 9
5016	F09[S-F]	Frequency of S – F at topological distance 9
5017	F09[S-Cl]	Frequency of S – Cl at topological distance 9
5018	F09[S-Br]	Frequency of S – Br at topological distance 9
5019	F09[S-I]	Frequency of S – I at topological distance 9
5020	F09[S-B]	Frequency of S – B at topological distance 9
5021	F09[S-Si]	Frequency of S – Si at topological distance 9
5022	F09[S-X]	Frequency of S – X at topological distance 9
5023	F09[P-P]	Frequency of P – P at topological distance 9
5024	F09[P-F]	Frequency of P – F at topological distance 9
5025	F09[P-Cl]	Frequency of P – Cl at topological distance 9
5026	F09[P-Br]	Frequency of P – Br at topological distance 9
5027	F09[P-I]	Frequency of P – I at topological distance 9
5028	F09[P-B]	Frequency of P – B at topological distance 9
5029	F09[P-Si]	Frequency of P – Si at topological distance 9
5030	F09[P-X]	Frequency of P – X at topological distance 9
5031	F09[F-F]	Frequency of F – F at topological distance 9
5032	F09[F-Cl]	Frequency of F – Cl at topological distance 9
5033	F09[F-Br]	Frequency of F – Br at topological distance 9
5034	F09[F-I]	Frequency of F – I at topological distance 9
5035	F09[F-B]	Frequency of F – B at topological distance 9
5036	F09[F-Si]	Frequency of F – Si at topological distance 9
5037	F09[F-X]	Frequency of F – X at topological distance 9
5038	F09[Cl-Cl]	Frequency of Cl – Cl at topological distance 9
5039	F09[Cl-Br]	Frequency of Cl – Br at topological distance 9
5040	F09[Cl-I]	Frequency of Cl – I at topological distance 9
5041	F09[Cl-B]	Frequency of Cl – B at topological distance 9
5042	F09[Cl-Si]	Frequency of Cl – Si at topological distance 9
5043	F09[Cl-X]	Frequency of Cl – X at topological distance 9
5044	F09[Br-Br]	Frequency of Br – Br at topological distance 9
5045	F09[Br-I]	Frequency of Br – I at topological distance 9
5046	F09[Br-B]	Frequency of Br – B at topological distance 9
5047	F09[Br-Si]	Frequency of Br – Si at topological distance 9
5048	F09[Br-X]	Frequency of Br – X at topological distance 9
5049	F09[I-I]	Frequency of I – I at topological distance 9

5050	F09[I-B]	Frequency of I – B at topological distance 9
5051	F09[I-Si]	Frequency of I – Si at topological distance 9
5052	F09[I-X]	Frequency of I – X at topological distance 9
5053	F09[B-B]	Frequency of B – B at topological distance 9
5054	F09[B-Si]	Frequency of B – Si at topological distance 9
5055	F09[B-X]	Frequency of B – X at topological distance 9
5056	F09[Si-Si]	Frequency of Si – Si at topological distance 9
5057	F09[Si-X]	Frequency of Si – X at topological distance 9
5058	F09[X-X]	Frequency of X – X at topological distance 9
5059	F10[C-C]	Frequency of C – C at topological distance 10
5060	F10[C-N]	Frequency of C – N at topological distance 10
5061	F10[C-O]	Frequency of C – O at topological distance 10
5062	F10[C-S]	Frequency of C – S at topological distance 10
5063	F10[C-P]	Frequency of C – P at topological distance 10
5064	F10[C-F]	Frequency of C – F at topological distance 10
5065	F10[C-Cl]	Frequency of C – Cl at topological distance 10
5066	F10[C-Br]	Frequency of C – Br at topological distance 10
5067	F10[C-I]	Frequency of C – I at topological distance 10
5068	F10[C-B]	Frequency of C – B at topological distance 10
5069	F10[C-Si]	Frequency of C – Si at topological distance 10
5070	F10[C-X]	Frequency of C – X at topological distance 10
5071	F10[N-N]	Frequency of N – N at topological distance 10
5072	F10[N-O]	Frequency of N – O at topological distance 10
5073	F10[N-S]	Frequency of N – S at topological distance 10
5074	F10[N-P]	Frequency of N – P at topological distance 10
5075	F10[N-F]	Frequency of N – F at topological distance 10
5076	F10[N-Cl]	Frequency of N – Cl at topological distance 10
5077	F10[N-Br]	Frequency of N – Br at topological distance 10
5078	F10[N-I]	Frequency of N – I at topological distance 10
5079	F10[N-B]	Frequency of N – B at topological distance 10
5080	F10[N-Si]	Frequency of N – Si at topological distance 10
5081	F10[N-X]	Frequency of N – X at topological distance 10
5082	F10[O-O]	Frequency of O – O at topological distance 10
5083	F10[O-S]	Frequency of O – S at topological distance 10
5084	F10[O-P]	Frequency of O – P at topological distance 10
5085	F10[O-F]	Frequency of O – F at topological distance 10
5086	F10[O-Cl]	Frequency of O – Cl at topological distance 10
5087	F10[O-Br]	Frequency of O – Br at topological distance 10
5088	F10[O-I]	Frequency of O – I at topological distance 10
5089	F10[O-B]	Frequency of O – B at topological distance 10
5090	F10[O-Si]	Frequency of O – Si at topological distance 10
5091	F10[O-X]	Frequency of O – X at topological distance 10

5092	F10[S-S]	Frequency of S – S at topological distance 10
5093	F10[S-P]	Frequency of S – P at topological distance 10
5094	F10[S-F]	Frequency of S – F at topological distance 10
5095	F10[S-Cl]	Frequency of S – Cl at topological distance 10
5096	F10[S-Br]	Frequency of S – Br at topological distance 10
5097	F10[S-I]	Frequency of S – I at topological distance 10
5098	F10[S-B]	Frequency of S – B at topological distance 10
5099	F10[S-Si]	Frequency of S – Si at topological distance 10
5100	F10[S-X]	Frequency of S – X at topological distance 10
5101	F10[P-P]	Frequency of P – P at topological distance 10
5102	F10[P-F]	Frequency of P – F at topological distance 10
5103	F10[P-Cl]	Frequency of P – Cl at topological distance 10
5104	F10[P-Br]	Frequency of P – Br at topological distance 10
5105	F10[P-I]	Frequency of P – I at topological distance 10
5106	F10[P-B]	Frequency of P – B at topological distance 10
5107	F10[P-Si]	Frequency of P – Si at topological distance 10
5108	F10[P-X]	Frequency of P – X at topological distance 10
5109	F10[F-F]	Frequency of F – F at topological distance 10
5110	F10[F-Cl]	Frequency of F – Cl at topological distance 10
5111	F10[F-Br]	Frequency of F – Br at topological distance 10
5112	F10[F-I]	Frequency of F – I at topological distance 10
5113	F10[F-B]	Frequency of F – B at topological distance 10
5114	F10[F-Si]	Frequency of F – Si at topological distance 10
5115	F10[F-X]	Frequency of F – X at topological distance 10
5116	F10[Cl-Cl]	Frequency of Cl – Cl at topological distance 10
5117	F10[Cl-Br]	Frequency of Cl – Br at topological distance 10
5118	F10[Cl-I]	Frequency of Cl – I at topological distance 10
5119	F10[Cl-B]	Frequency of Cl – B at topological distance 10
5120	F10[Cl-Si]	Frequency of Cl – Si at topological distance 10
5121	F10[Cl-X]	Frequency of Cl – X at topological distance 10
5122	F10[Br-Br]	Frequency of Br – Br at topological distance 10
5123	F10[Br-I]	Frequency of Br – I at topological distance 10
5124	F10[Br-B]	Frequency of Br – B at topological distance 10
5125	F10[Br-Si]	Frequency of Br – Si at topological distance 10
5126	F10[Br-X]	Frequency of Br – X at topological distance 10
5127	F10[I-I]	Frequency of I – I at topological distance 10
5128	F10[I-B]	Frequency of I – B at topological distance 10
5129	F10[I-Si]	Frequency of I – Si at topological distance 10
5130	F10[I-X]	Frequency of I – X at topological distance 10
5131	F10[B-B]	Frequency of B – B at topological distance 10
5132	F10[B-Si]	Frequency of B – Si at topological distance 10
5133	F10[B-X]	Frequency of B – X at topological distance 10

5134	F10[Si-Si]	Frequency of Si – Si at topological distance 10
5135	F10[Si-X]	Frequency of Si – X at topological distance 10
5136	F10[X-X]	Frequency of X – X at topological distance 10

26. 3D Atom Pairs

No.	Name	Description
5137	G(N..N)	sum of geometrical distances between N..N
5138	G(N..O)	sum of geometrical distances between N..O
5139	G(N..S)	sum of geometrical distances between N..S
5140	G(N..P)	sum of geometrical distances between N..P
5141	G(N..F)	sum of geometrical distances between N..F
5142	G(N..Cl)	sum of geometrical distances between N..Cl
5143	G(N..Br)	sum of geometrical distances between N..Br
5144	G(N..I)	sum of geometrical distances between N..I
5145	G(O..O)	sum of geometrical distances between O..O
5146	G(O..S)	sum of geometrical distances between O..S
5147	G(O..P)	sum of geometrical distances between O..P
5148	G(O..F)	sum of geometrical distances between O..F
5149	G(O..Cl)	sum of geometrical distances between O..Cl
5150	G(O..Br)	sum of geometrical distances between O..Br
5151	G(O..I)	sum of geometrical distances between O..I
5152	G(S..S)	sum of geometrical distances between S..S
5153	G(S..P)	sum of geometrical distances between S..P
5154	G(S..F)	sum of geometrical distances between S..F
5155	G(S..Cl)	sum of geometrical distances between S..Cl
5156	G(S..Br)	sum of geometrical distances between S..Br
5157	G(S..I)	sum of geometrical distances between S..I
5158	G(P..P)	sum of geometrical distances between P..P
5159	G(P..F)	sum of geometrical distances between P..F
5160	G(P..Cl)	sum of geometrical distances between P..Cl
5161	G(P..Br)	sum of geometrical distances between P..Br
5162	G(P..I)	sum of geometrical distances between P..I
5163	G(F..F)	sum of geometrical distances between F..F
5164	G(F..Cl)	sum of geometrical distances between F..Cl
5165	G(F..Br)	sum of geometrical distances between F..Br
5166	G(F..I)	sum of geometrical distances between F..I
5167	G(Cl..Cl)	sum of geometrical distances between Cl..Cl
5168	G(Cl..Br)	sum of geometrical distances between Cl..Br
5169	G(Cl..I)	sum of geometrical distances between Cl..I
5170	G(Br..Br)	sum of geometrical distances between Br..Br
5171	G(Br..I)	sum of geometrical distances between Br..I
5172	G(I..I)	sum of geometrical distances between I..I

27. Charge descriptors

No.	Name	Description
5173	qpmax	maximum positive charge
5174	qnmax	maximum negative charge
5175	Qpos	total positive charge
5176	Qneg	total negative charge
5177	Qtot	total absolute charge (electronic charge index – ECI)
5178	Qmean	mean absolute charge (charge polarization)
5179	Q2	total squared charge
5180	RPCG	relative positive charge
5181	RNCG	relative negative charge
5182	SPP	submolecular polarity parameter
5183	TE1	topographic electronic descriptor
5184	TE2	topographic electronic descriptor (bond resctricted)
5185	PCWTE1	partial charge weighted topological electronic index
5186	PCWTE2	partial charge weighted topological electronic index (bond resctricted)
5187	LDI	local dipole index

28. Molecular properties

No.	Name	Description
5188	Uc	unsaturation count
5189	Ui	unsaturation index
5190	Hy	hydrophilic factor
5191	AMR	Ghose-Crippen molar refractivity
5192	MR99	Wildmann-Crippen molar refractivity
5193	MRcons	Molar refractivity (consensus)
5194	TPSA(NO)	topological polar surface area using N,O polar contributions
5195	TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions
5196	MLOGP	Moriguchi octanol-water partition coeff. (logP)
5197	MLOGP2	squared Moriguchi octanol-water partition coeff. (logP^2)
5198	ALOGP	Ghose-Crippen octanol-water partition coeff. (logP)
5199	ALOGP2	squared Ghose-Crippen octanol-water partition coeff. (logP^2)
5200	LOGP99	Wildmann-Crippen octanol-water partition coeff. (logP)
5201	LOGPcons	Octanol-water partition coeff. (logP) (consensus)
5202	ESOL	Estimated SOLubility (logS) for aqueous solubility using LOGPcons
5203	SAtot	total surface area from P_VSA-like descriptors
5204	SAacc	surface area of acceptor atoms from P_VSA-like descriptors
5205	SAdon	surface area of donor atoms from P_VSA-like descriptors
5206	Vx	McGowan volume
5207	VvdwMG	van der Waals volume from McGowan volume
5208	VvdwZAZ	van der Waals volume from Zhao-Abraham-Zissimos equation
5209	PDI	packing density index

5210	BLTF96	Verhaar Fish base-line toxicity from MLOGP (mmol/l)
5211	BLTD48	Verhaar Daphnia base-line toxicity from MLOGP (mmol/l)
5212	BLTA96	Verhaar Algae base-line toxicity from MLOGP (mmol/l)
5213	SAscore	Synthetic Accessibility score
5214	PBF	Plane of best fit

29. Drug-like indices

No.	Name	Description
5215	Ro5	Lipinski Rule of 5
5216	cRo5	Complementary Lipinski Alert index
5217	DLS_01	modified drug-like score from Lipinski (4 rules)
5218	DLS_02	modified drug-like score from Oprea et al. (6 rules)
5219	DLS_03	modified drug-like score from Walters et al. (6 rules)
5220	DLS_04	modified drug-like score from Chen et al. (7 rules)
5221	DLS_05	modified drug-like score from Zheng et al. (2 rules)
5222	DLS_06	modified drug-like score from Rishton (6 rules)
5223	DLS_07	modified drug-like score from Veber et al. (2 rules)
5224	DLS_cons	DRAGON consensus drug-like score
5225	LLS_01	modified lead-like score from Congreve et al. (6 rules) – (rule of three (Ro3))
5226	LLS_02	modified lead-like score from Monge et al. (8 rules)
5227	CMC-80	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 80%
5228	CMC-50	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 50%
5229	Inflammat-80	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80%
5230	Inflammat-50	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50%
5231	Depressant-80	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80%
5232	Depressant-50	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50%
5233	Psychotic-80	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80%
5234	Psychotic-50	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50%
5235	Hypertens-80	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80%
5236	Hypertens-50	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50%
5237	Hypnotic-80	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80%
5238	Hypnotic-50	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50%
5239	Neoplastic-80	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80%
5240	Neoplastic-50	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50%
5241	Infective-80	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80%
5242	Infective-50	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50%
5243	QEDu	Quantitative Estimation of Drug-likeness (unweighted)
5244	QED	Quantitative Estimation of Drug-likeness

30. CATS 3D descriptors

No.	Name	Description
5245	CATS3D_00_DD	CATS3D Donor-Donor BIN 00 (0.000 – 1.000 Å)
5246	CATS3D_01_DD	CATS3D Donor-Donor BIN 01 (1.000 – 2.000 Å)

5247	CATS3D_02_DD	CATS3D Donor-Donor BIN 02 (2.000 – 3.000 Å)
5248	CATS3D_03_DD	CATS3D Donor-Donor BIN 03 (3.000 – 4.000 Å)
5249	CATS3D_04_DD	CATS3D Donor-Donor BIN 04 (4.000 – 5.000 Å)
5250	CATS3D_05_DD	CATS3D Donor-Donor BIN 05 (5.000 – 6.000 Å)
5251	CATS3D_06_DD	CATS3D Donor-Donor BIN 06 (6.000 – 7.000 Å)
5252	CATS3D_07_DD	CATS3D Donor-Donor BIN 07 (7.000 – 8.000 Å)
5253	CATS3D_08_DD	CATS3D Donor-Donor BIN 08 (8.000 – 9.000 Å)
5254	CATS3D_09_DD	CATS3D Donor-Donor BIN 09 (9.000 – 10.000 Å)
5255	CATS3D_10_DD	CATS3D Donor-Donor BIN 10 (10.000 – 11.000 Å)
5256	CATS3D_11_DD	CATS3D Donor-Donor BIN 11 (11.000 – 12.000 Å)
5257	CATS3D_12_DD	CATS3D Donor-Donor BIN 12 (12.000 – 13.000 Å)
5258	CATS3D_13_DD	CATS3D Donor-Donor BIN 13 (13.000 – 14.000 Å)
5259	CATS3D_14_DD	CATS3D Donor-Donor BIN 14 (14.000 – 15.000 Å)
5260	CATS3D_15_DD	CATS3D Donor-Donor BIN 15 (15.000 – 16.000 Å)
5261	CATS3D_16_DD	CATS3D Donor-Donor BIN 16 (16.000 – 17.000 Å)
5262	CATS3D_17_DD	CATS3D Donor-Donor BIN 17 (17.000 – 18.000 Å)
5263	CATS3D_18_DD	CATS3D Donor-Donor BIN 18 (18.000 – 19.000 Å)
5264	CATS3D_19_DD	CATS3D Donor-Donor BIN 19 (19.000 – 20.000 Å)
5265	CATS3D_00_DA	CATS3D Donor-Acceptor BIN 00 (0.000 – 1.000 Å)
5266	CATS3D_01_DA	CATS3D Donor-Acceptor BIN 01 (1.000 – 2.000 Å)
5267	CATS3D_02_DA	CATS3D Donor-Acceptor BIN 02 (2.000 – 3.000 Å)
5268	CATS3D_03_DA	CATS3D Donor-Acceptor BIN 03 (3.000 – 4.000 Å)
5269	CATS3D_04_DA	CATS3D Donor-Acceptor BIN 04 (4.000 – 5.000 Å)
5270	CATS3D_05_DA	CATS3D Donor-Acceptor BIN 05 (5.000 – 6.000 Å)
5271	CATS3D_06_DA	CATS3D Donor-Acceptor BIN 06 (6.000 – 7.000 Å)
5272	CATS3D_07_DA	CATS3D Donor-Acceptor BIN 07 (7.000 – 8.000 Å)
5273	CATS3D_08_DA	CATS3D Donor-Acceptor BIN 08 (8.000 – 9.000 Å)
5274	CATS3D_09_DA	CATS3D Donor-Acceptor BIN 09 (9.000 – 10.000 Å)
5275	CATS3D_10_DA	CATS3D Donor-Acceptor BIN 10 (10.000 – 11.000 Å)
5276	CATS3D_11_DA	CATS3D Donor-Acceptor BIN 11 (11.000 – 12.000 Å)
5277	CATS3D_12_DA	CATS3D Donor-Acceptor BIN 12 (12.000 – 13.000 Å)
5278	CATS3D_13_DA	CATS3D Donor-Acceptor BIN 13 (13.000 – 14.000 Å)
5279	CATS3D_14_DA	CATS3D Donor-Acceptor BIN 14 (14.000 – 15.000 Å)
5280	CATS3D_15_DA	CATS3D Donor-Acceptor BIN 15 (15.000 – 16.000 Å)
5281	CATS3D_16_DA	CATS3D Donor-Acceptor BIN 16 (16.000 – 17.000 Å)
5282	CATS3D_17_DA	CATS3D Donor-Acceptor BIN 17 (17.000 – 18.000 Å)
5283	CATS3D_18_DA	CATS3D Donor-Acceptor BIN 18 (18.000 – 19.000 Å)
5284	CATS3D_19_DA	CATS3D Donor-Acceptor BIN 19 (19.000 – 20.000 Å)
5285	CATS3D_00_DP	CATS3D Donor-Positive BIN 00 (0.000 – 1.000 Å)
5286	CATS3D_01_DP	CATS3D Donor-Positive BIN 01 (1.000 – 2.000 Å)
5287	CATS3D_02_DP	CATS3D Donor-Positive BIN 02 (2.000 – 3.000 Å)
5288	CATS3D_03_DP	CATS3D Donor-Positive BIN 03 (3.000 – 4.000 Å)

5289	CATS3D_04_DP	CATS3D Donor-Positive BIN 04 (4.000 – 5.000 Å)
5290	CATS3D_05_DP	CATS3D Donor-Positive BIN 05 (5.000 – 6.000 Å)
5291	CATS3D_06_DP	CATS3D Donor-Positive BIN 06 (6.000 – 7.000 Å)
5292	CATS3D_07_DP	CATS3D Donor-Positive BIN 07 (7.000 – 8.000 Å)
5293	CATS3D_08_DP	CATS3D Donor-Positive BIN 08 (8.000 – 9.000 Å)
5294	CATS3D_09_DP	CATS3D Donor-Positive BIN 09 (9.000 – 10.000 Å)
5295	CATS3D_10_DP	CATS3D Donor-Positive BIN 10 (10.000 – 11.000 Å)
5296	CATS3D_11_DP	CATS3D Donor-Positive BIN 11 (11.000 – 12.000 Å)
5297	CATS3D_12_DP	CATS3D Donor-Positive BIN 12 (12.000 – 13.000 Å)
5298	CATS3D_13_DP	CATS3D Donor-Positive BIN 13 (13.000 – 14.000 Å)
5299	CATS3D_14_DP	CATS3D Donor-Positive BIN 14 (14.000 – 15.000 Å)
5300	CATS3D_15_DP	CATS3D Donor-Positive BIN 15 (15.000 – 16.000 Å)
5301	CATS3D_16_DP	CATS3D Donor-Positive BIN 16 (16.000 – 17.000 Å)
5302	CATS3D_17_DP	CATS3D Donor-Positive BIN 17 (17.000 – 18.000 Å)
5303	CATS3D_18_DP	CATS3D Donor-Positive BIN 18 (18.000 – 19.000 Å)
5304	CATS3D_19_DP	CATS3D Donor-Positive BIN 19 (19.000 – 20.000 Å)
5305	CATS3D_00_DN	CATS3D Donor-Negative BIN 00 (0.000 – 1.000 Å)
5306	CATS3D_01_DN	CATS3D Donor-Negative BIN 01 (1.000 – 2.000 Å)
5307	CATS3D_02_DN	CATS3D Donor-Negative BIN 02 (2.000 – 3.000 Å)
5308	CATS3D_03_DN	CATS3D Donor-Negative BIN 03 (3.000 – 4.000 Å)
5309	CATS3D_04_DN	CATS3D Donor-Negative BIN 04 (4.000 – 5.000 Å)
5310	CATS3D_05_DN	CATS3D Donor-Negative BIN 05 (5.000 – 6.000 Å)
5311	CATS3D_06_DN	CATS3D Donor-Negative BIN 06 (6.000 – 7.000 Å)
5312	CATS3D_07_DN	CATS3D Donor-Negative BIN 07 (7.000 – 8.000 Å)
5313	CATS3D_08_DN	CATS3D Donor-Negative BIN 08 (8.000 – 9.000 Å)
5314	CATS3D_09_DN	CATS3D Donor-Negative BIN 09 (9.000 – 10.000 Å)
5315	CATS3D_10_DN	CATS3D Donor-Negative BIN 10 (10.000 – 11.000 Å)
5316	CATS3D_11_DN	CATS3D Donor-Negative BIN 11 (11.000 – 12.000 Å)
5317	CATS3D_12_DN	CATS3D Donor-Negative BIN 12 (12.000 – 13.000 Å)
5318	CATS3D_13_DN	CATS3D Donor-Negative BIN 13 (13.000 – 14.000 Å)
5319	CATS3D_14_DN	CATS3D Donor-Negative BIN 14 (14.000 – 15.000 Å)
5320	CATS3D_15_DN	CATS3D Donor-Negative BIN 15 (15.000 – 16.000 Å)
5321	CATS3D_16_DN	CATS3D Donor-Negative BIN 16 (16.000 – 17.000 Å)
5322	CATS3D_17_DN	CATS3D Donor-Negative BIN 17 (17.000 – 18.000 Å)
5323	CATS3D_18_DN	CATS3D Donor-Negative BIN 18 (18.000 – 19.000 Å)
5324	CATS3D_19_DN	CATS3D Donor-Negative BIN 19 (19.000 – 20.000 Å)
5325	CATS3D_00_DL	CATS3D Donor-Lipophilic BIN 00 (0.000 – 1.000 Å)
5326	CATS3D_01_DL	CATS3D Donor-Lipophilic BIN 01 (1.000 – 2.000 Å)
5327	CATS3D_02_DL	CATS3D Donor-Lipophilic BIN 02 (2.000 – 3.000 Å)
5328	CATS3D_03_DL	CATS3D Donor-Lipophilic BIN 03 (3.000 – 4.000 Å)
5329	CATS3D_04_DL	CATS3D Donor-Lipophilic BIN 04 (4.000 – 5.000 Å)
5330	CATS3D_05_DL	CATS3D Donor-Lipophilic BIN 05 (5.000 – 6.000 Å)

5331	CATS3D_06_DL	CATS3D Donor-Lipophilic BIN 06 (6.000 – 7.000 Å)
5332	CATS3D_07_DL	CATS3D Donor-Lipophilic BIN 07 (7.000 – 8.000 Å)
5333	CATS3D_08_DL	CATS3D Donor-Lipophilic BIN 08 (8.000 – 9.000 Å)
5334	CATS3D_09_DL	CATS3D Donor-Lipophilic BIN 09 (9.000 – 10.000 Å)
5335	CATS3D_10_DL	CATS3D Donor-Lipophilic BIN 10 (10.000 – 11.000 Å)
5336	CATS3D_11_DL	CATS3D Donor-Lipophilic BIN 11 (11.000 – 12.000 Å)
5337	CATS3D_12_DL	CATS3D Donor-Lipophilic BIN 12 (12.000 – 13.000 Å)
5338	CATS3D_13_DL	CATS3D Donor-Lipophilic BIN 13 (13.000 – 14.000 Å)
5339	CATS3D_14_DL	CATS3D Donor-Lipophilic BIN 14 (14.000 – 15.000 Å)
5340	CATS3D_15_DL	CATS3D Donor-Lipophilic BIN 15 (15.000 – 16.000 Å)
5341	CATS3D_16_DL	CATS3D Donor-Lipophilic BIN 16 (16.000 – 17.000 Å)
5342	CATS3D_17_DL	CATS3D Donor-Lipophilic BIN 17 (17.000 – 18.000 Å)
5343	CATS3D_18_DL	CATS3D Donor-Lipophilic BIN 18 (18.000 – 19.000 Å)
5344	CATS3D_19_DL	CATS3D Donor-Lipophilic BIN 19 (19.000 – 20.000 Å)
5345	CATS3D_00_AA	CATS3D Acceptor-Acceptor BIN 00 (0.000 – 1.000 Å)
5346	CATS3D_01_AA	CATS3D Acceptor-Acceptor BIN 01 (1.000 – 2.000 Å)
5347	CATS3D_02_AA	CATS3D Acceptor-Acceptor BIN 02 (2.000 – 3.000 Å)
5348	CATS3D_03_AA	CATS3D Acceptor-Acceptor BIN 03 (3.000 – 4.000 Å)
5349	CATS3D_04_AA	CATS3D Acceptor-Acceptor BIN 04 (4.000 – 5.000 Å)
5350	CATS3D_05_AA	CATS3D Acceptor-Acceptor BIN 05 (5.000 – 6.000 Å)
5351	CATS3D_06_AA	CATS3D Acceptor-Acceptor BIN 06 (6.000 – 7.000 Å)
5352	CATS3D_07_AA	CATS3D Acceptor-Acceptor BIN 07 (7.000 – 8.000 Å)
5353	CATS3D_08_AA	CATS3D Acceptor-Acceptor BIN 08 (8.000 – 9.000 Å)
5354	CATS3D_09_AA	CATS3D Acceptor-Acceptor BIN 09 (9.000 – 10.000 Å)
5355	CATS3D_10_AA	CATS3D Acceptor-Acceptor BIN 10 (10.000 – 11.000 Å)
5356	CATS3D_11_AA	CATS3D Acceptor-Acceptor BIN 11 (11.000 – 12.000 Å)
5357	CATS3D_12_AA	CATS3D Acceptor-Acceptor BIN 12 (12.000 – 13.000 Å)
5358	CATS3D_13_AA	CATS3D Acceptor-Acceptor BIN 13 (13.000 – 14.000 Å)
5359	CATS3D_14_AA	CATS3D Acceptor-Acceptor BIN 14 (14.000 – 15.000 Å)
5360	CATS3D_15_AA	CATS3D Acceptor-Acceptor BIN 15 (15.000 – 16.000 Å)
5361	CATS3D_16_AA	CATS3D Acceptor-Acceptor BIN 16 (16.000 – 17.000 Å)
5362	CATS3D_17_AA	CATS3D Acceptor-Acceptor BIN 17 (17.000 – 18.000 Å)
5363	CATS3D_18_AA	CATS3D Acceptor-Acceptor BIN 18 (18.000 – 19.000 Å)
5364	CATS3D_19_AA	CATS3D Acceptor-Acceptor BIN 19 (19.000 – 20.000 Å)
5365	CATS3D_00_AP	CATS3D Acceptor-Positive BIN 00 (0.000 – 1.000 Å)
5366	CATS3D_01_AP	CATS3D Acceptor-Positive BIN 01 (1.000 – 2.000 Å)
5367	CATS3D_02_AP	CATS3D Acceptor-Positive BIN 02 (2.000 – 3.000 Å)
5368	CATS3D_03_AP	CATS3D Acceptor-Positive BIN 03 (3.000 – 4.000 Å)
5369	CATS3D_04_AP	CATS3D Acceptor-Positive BIN 04 (4.000 – 5.000 Å)
5370	CATS3D_05_AP	CATS3D Acceptor-Positive BIN 05 (5.000 – 6.000 Å)
5371	CATS3D_06_AP	CATS3D Acceptor-Positive BIN 06 (6.000 – 7.000 Å)
5372	CATS3D_07_AP	CATS3D Acceptor-Positive BIN 07 (7.000 – 8.000 Å)

5373	CATS3D_08_AP	CATS3D Acceptor-Positive BIN 08 (8.000 – 9.000 Å)
5374	CATS3D_09_AP	CATS3D Acceptor-Positive BIN 09 (9.000 – 10.000 Å)
5375	CATS3D_10_AP	CATS3D Acceptor-Positive BIN 10 (10.000 – 11.000 Å)
5376	CATS3D_11_AP	CATS3D Acceptor-Positive BIN 11 (11.000 – 12.000 Å)
5377	CATS3D_12_AP	CATS3D Acceptor-Positive BIN 12 (12.000 – 13.000 Å)
5378	CATS3D_13_AP	CATS3D Acceptor-Positive BIN 13 (13.000 – 14.000 Å)
5379	CATS3D_14_AP	CATS3D Acceptor-Positive BIN 14 (14.000 – 15.000 Å)
5380	CATS3D_15_AP	CATS3D Acceptor-Positive BIN 15 (15.000 – 16.000 Å)
5381	CATS3D_16_AP	CATS3D Acceptor-Positive BIN 16 (16.000 – 17.000 Å)
5382	CATS3D_17_AP	CATS3D Acceptor-Positive BIN 17 (17.000 – 18.000 Å)
5383	CATS3D_18_AP	CATS3D Acceptor-Positive BIN 18 (18.000 – 19.000 Å)
5384	CATS3D_19_AP	CATS3D Acceptor-Positive BIN 19 (19.000 – 20.000 Å)
5385	CATS3D_00_AN	CATS3D Acceptor-Negative BIN 00 (0.000 – 1.000 Å)
5386	CATS3D_01_AN	CATS3D Acceptor-Negative BIN 01 (1.000 – 2.000 Å)
5387	CATS3D_02_AN	CATS3D Acceptor-Negative BIN 02 (2.000 – 3.000 Å)
5388	CATS3D_03_AN	CATS3D Acceptor-Negative BIN 03 (3.000 – 4.000 Å)
5389	CATS3D_04_AN	CATS3D Acceptor-Negative BIN 04 (4.000 – 5.000 Å)
5390	CATS3D_05_AN	CATS3D Acceptor-Negative BIN 05 (5.000 – 6.000 Å)
5391	CATS3D_06_AN	CATS3D Acceptor-Negative BIN 06 (6.000 – 7.000 Å)
5392	CATS3D_07_AN	CATS3D Acceptor-Negative BIN 07 (7.000 – 8.000 Å)
5393	CATS3D_08_AN	CATS3D Acceptor-Negative BIN 08 (8.000 – 9.000 Å)
5394	CATS3D_09_AN	CATS3D Acceptor-Negative BIN 09 (9.000 – 10.000 Å)
5395	CATS3D_10_AN	CATS3D Acceptor-Negative BIN 10 (10.000 – 11.000 Å)
5396	CATS3D_11_AN	CATS3D Acceptor-Negative BIN 11 (11.000 – 12.000 Å)
5397	CATS3D_12_AN	CATS3D Acceptor-Negative BIN 12 (12.000 – 13.000 Å)
5398	CATS3D_13_AN	CATS3D Acceptor-Negative BIN 13 (13.000 – 14.000 Å)
5399	CATS3D_14_AN	CATS3D Acceptor-Negative BIN 14 (14.000 – 15.000 Å)
5400	CATS3D_15_AN	CATS3D Acceptor-Negative BIN 15 (15.000 – 16.000 Å)
5401	CATS3D_16_AN	CATS3D Acceptor-Negative BIN 16 (16.000 – 17.000 Å)
5402	CATS3D_17_AN	CATS3D Acceptor-Negative BIN 17 (17.000 – 18.000 Å)
5403	CATS3D_18_AN	CATS3D Acceptor-Negative BIN 18 (18.000 – 19.000 Å)
5404	CATS3D_19_AN	CATS3D Acceptor-Negative BIN 19 (19.000 – 20.000 Å)
5405	CATS3D_00_AL	CATS3D Acceptor-Lipophilic BIN 00 (0.000 – 1.000 Å)
5406	CATS3D_01_AL	CATS3D Acceptor-Lipophilic BIN 01 (1.000 – 2.000 Å)
5407	CATS3D_02_AL	CATS3D Acceptor-Lipophilic BIN 02 (2.000 – 3.000 Å)
5408	CATS3D_03_AL	CATS3D Acceptor-Lipophilic BIN 03 (3.000 – 4.000 Å)
5409	CATS3D_04_AL	CATS3D Acceptor-Lipophilic BIN 04 (4.000 – 5.000 Å)
5410	CATS3D_05_AL	CATS3D Acceptor-Lipophilic BIN 05 (5.000 – 6.000 Å)
5411	CATS3D_06_AL	CATS3D Acceptor-Lipophilic BIN 06 (6.000 – 7.000 Å)
5412	CATS3D_07_AL	CATS3D Acceptor-Lipophilic BIN 07 (7.000 – 8.000 Å)
5413	CATS3D_08_AL	CATS3D Acceptor-Lipophilic BIN 08 (8.000 – 9.000 Å)
5414	CATS3D_09_AL	CATS3D Acceptor-Lipophilic BIN 09 (9.000 – 10.000 Å)

5415	CATS3D_10_AL	CATS3D Acceptor-Lipophilic BIN 10 (10.000 – 11.000 Å)
5416	CATS3D_11_AL	CATS3D Acceptor-Lipophilic BIN 11 (11.000 – 12.000 Å)
5417	CATS3D_12_AL	CATS3D Acceptor-Lipophilic BIN 12 (12.000 – 13.000 Å)
5418	CATS3D_13_AL	CATS3D Acceptor-Lipophilic BIN 13 (13.000 – 14.000 Å)
5419	CATS3D_14_AL	CATS3D Acceptor-Lipophilic BIN 14 (14.000 – 15.000 Å)
5420	CATS3D_15_AL	CATS3D Acceptor-Lipophilic BIN 15 (15.000 – 16.000 Å)
5421	CATS3D_16_AL	CATS3D Acceptor-Lipophilic BIN 16 (16.000 – 17.000 Å)
5422	CATS3D_17_AL	CATS3D Acceptor-Lipophilic BIN 17 (17.000 – 18.000 Å)
5423	CATS3D_18_AL	CATS3D Acceptor-Lipophilic BIN 18 (18.000 – 19.000 Å)
5424	CATS3D_19_AL	CATS3D Acceptor-Lipophilic BIN 19 (19.000 – 20.000 Å)
5425	CATS3D_00_PP	CATS3D Positive-Positive BIN 00 (0.000 – 1.000 Å)
5426	CATS3D_01_PP	CATS3D Positive-Positive BIN 01 (1.000 – 2.000 Å)
5427	CATS3D_02_PP	CATS3D Positive-Positive BIN 02 (2.000 – 3.000 Å)
5428	CATS3D_03_PP	CATS3D Positive-Positive BIN 03 (3.000 – 4.000 Å)
5429	CATS3D_04_PP	CATS3D Positive-Positive BIN 04 (4.000 – 5.000 Å)
5430	CATS3D_05_PP	CATS3D Positive-Positive BIN 05 (5.000 – 6.000 Å)
5431	CATS3D_06_PP	CATS3D Positive-Positive BIN 06 (6.000 – 7.000 Å)
5432	CATS3D_07_PP	CATS3D Positive-Positive BIN 07 (7.000 – 8.000 Å)
5433	CATS3D_08_PP	CATS3D Positive-Positive BIN 08 (8.000 – 9.000 Å)
5434	CATS3D_09_PP	CATS3D Positive-Positive BIN 09 (9.000 – 10.000 Å)
5435	CATS3D_10_PP	CATS3D Positive-Positive BIN 10 (10.000 – 11.000 Å)
5436	CATS3D_11_PP	CATS3D Positive-Positive BIN 11 (11.000 – 12.000 Å)
5437	CATS3D_12_PP	CATS3D Positive-Positive BIN 12 (12.000 – 13.000 Å)
5438	CATS3D_13_PP	CATS3D Positive-Positive BIN 13 (13.000 – 14.000 Å)
5439	CATS3D_14_PP	CATS3D Positive-Positive BIN 14 (14.000 – 15.000 Å)
5440	CATS3D_15_PP	CATS3D Positive-Positive BIN 15 (15.000 – 16.000 Å)
5441	CATS3D_16_PP	CATS3D Positive-Positive BIN 16 (16.000 – 17.000 Å)
5442	CATS3D_17_PP	CATS3D Positive-Positive BIN 17 (17.000 – 18.000 Å)
5443	CATS3D_18_PP	CATS3D Positive-Positive BIN 18 (18.000 – 19.000 Å)
5444	CATS3D_19_PP	CATS3D Positive-Positive BIN 19 (19.000 – 20.000 Å)
5445	CATS3D_00_PN	CATS3D Positive-Negative BIN 00 (0.000 – 1.000 Å)
5446	CATS3D_01_PN	CATS3D Positive-Negative BIN 01 (1.000 – 2.000 Å)
5447	CATS3D_02_PN	CATS3D Positive-Negative BIN 02 (2.000 – 3.000 Å)
5448	CATS3D_03_PN	CATS3D Positive-Negative BIN 03 (3.000 – 4.000 Å)
5449	CATS3D_04_PN	CATS3D Positive-Negative BIN 04 (4.000 – 5.000 Å)
5450	CATS3D_05_PN	CATS3D Positive-Negative BIN 05 (5.000 – 6.000 Å)
5451	CATS3D_06_PN	CATS3D Positive-Negative BIN 06 (6.000 – 7.000 Å)
5452	CATS3D_07_PN	CATS3D Positive-Negative BIN 07 (7.000 – 8.000 Å)
5453	CATS3D_08_PN	CATS3D Positive-Negative BIN 08 (8.000 – 9.000 Å)
5454	CATS3D_09_PN	CATS3D Positive-Negative BIN 09 (9.000 – 10.000 Å)
5455	CATS3D_10_PN	CATS3D Positive-Negative BIN 10 (10.000 – 11.000 Å)
5456	CATS3D_11_PN	CATS3D Positive-Negative BIN 11 (11.000 – 12.000 Å)

5457	CATS3D_12_PN	CATS3D Positive-Negative BIN 12 (12.000 – 13.000 Å)
5458	CATS3D_13_PN	CATS3D Positive-Negative BIN 13 (13.000 – 14.000 Å)
5459	CATS3D_14_PN	CATS3D Positive-Negative BIN 14 (14.000 – 15.000 Å)
5460	CATS3D_15_PN	CATS3D Positive-Negative BIN 15 (15.000 – 16.000 Å)
5461	CATS3D_16_PN	CATS3D Positive-Negative BIN 16 (16.000 – 17.000 Å)
5462	CATS3D_17_PN	CATS3D Positive-Negative BIN 17 (17.000 – 18.000 Å)
5463	CATS3D_18_PN	CATS3D Positive-Negative BIN 18 (18.000 – 19.000 Å)
5464	CATS3D_19_PN	CATS3D Positive-Negative BIN 19 (19.000 – 20.000 Å)
5465	CATS3D_00_PL	CATS3D Positive-Lipophilic BIN 00 (0.000 – 1.000 Å)
5466	CATS3D_01_PL	CATS3D Positive-Lipophilic BIN 01 (1.000 – 2.000 Å)
5467	CATS3D_02_PL	CATS3D Positive-Lipophilic BIN 02 (2.000 – 3.000 Å)
5468	CATS3D_03_PL	CATS3D Positive-Lipophilic BIN 03 (3.000 – 4.000 Å)
5469	CATS3D_04_PL	CATS3D Positive-Lipophilic BIN 04 (4.000 – 5.000 Å)
5470	CATS3D_05_PL	CATS3D Positive-Lipophilic BIN 05 (5.000 – 6.000 Å)
5471	CATS3D_06_PL	CATS3D Positive-Lipophilic BIN 06 (6.000 – 7.000 Å)
5472	CATS3D_07_PL	CATS3D Positive-Lipophilic BIN 07 (7.000 – 8.000 Å)
5473	CATS3D_08_PL	CATS3D Positive-Lipophilic BIN 08 (8.000 – 9.000 Å)
5474	CATS3D_09_PL	CATS3D Positive-Lipophilic BIN 09 (9.000 – 10.000 Å)
5475	CATS3D_10_PL	CATS3D Positive-Lipophilic BIN 10 (10.000 – 11.000 Å)
5476	CATS3D_11_PL	CATS3D Positive-Lipophilic BIN 11 (11.000 – 12.000 Å)
5477	CATS3D_12_PL	CATS3D Positive-Lipophilic BIN 12 (12.000 – 13.000 Å)
5478	CATS3D_13_PL	CATS3D Positive-Lipophilic BIN 13 (13.000 – 14.000 Å)
5479	CATS3D_14_PL	CATS3D Positive-Lipophilic BIN 14 (14.000 – 15.000 Å)
5480	CATS3D_15_PL	CATS3D Positive-Lipophilic BIN 15 (15.000 – 16.000 Å)
5481	CATS3D_16_PL	CATS3D Positive-Lipophilic BIN 16 (16.000 – 17.000 Å)
5482	CATS3D_17_PL	CATS3D Positive-Lipophilic BIN 17 (17.000 – 18.000 Å)
5483	CATS3D_18_PL	CATS3D Positive-Lipophilic BIN 18 (18.000 – 19.000 Å)
5484	CATS3D_19_PL	CATS3D Positive-Lipophilic BIN 19 (19.000 – 20.000 Å)
5485	CATS3D_00_NN	CATS3D Negative-Negative BIN 00 (0.000 – 1.000 Å)
5486	CATS3D_01_NN	CATS3D Negative-Negative BIN 01 (1.000 – 2.000 Å)
5487	CATS3D_02_NN	CATS3D Negative-Negative BIN 02 (2.000 – 3.000 Å)
5488	CATS3D_03_NN	CATS3D Negative-Negative BIN 03 (3.000 – 4.000 Å)
5489	CATS3D_04_NN	CATS3D Negative-Negative BIN 04 (4.000 – 5.000 Å)
5490	CATS3D_05_NN	CATS3D Negative-Negative BIN 05 (5.000 – 6.000 Å)
5491	CATS3D_06_NN	CATS3D Negative-Negative BIN 06 (6.000 – 7.000 Å)
5492	CATS3D_07_NN	CATS3D Negative-Negative BIN 07 (7.000 – 8.000 Å)
5493	CATS3D_08_NN	CATS3D Negative-Negative BIN 08 (8.000 – 9.000 Å)
5494	CATS3D_09_NN	CATS3D Negative-Negative BIN 09 (9.000 – 10.000 Å)
5495	CATS3D_10_NN	CATS3D Negative-Negative BIN 10 (10.000 – 11.000 Å)
5496	CATS3D_11_NN	CATS3D Negative-Negative BIN 11 (11.000 – 12.000 Å)
5497	CATS3D_12_NN	CATS3D Negative-Negative BIN 12 (12.000 – 13.000 Å)
5498	CATS3D_13_NN	CATS3D Negative-Negative BIN 13 (13.000 – 14.000 Å)

5499	CATS3D_14_NN	CATS3D Negative-Negative BIN 14 (14.000 – 15.000 Å)
5500	CATS3D_15_NN	CATS3D Negative-Negative BIN 15 (15.000 – 16.000 Å)
5501	CATS3D_16_NN	CATS3D Negative-Negative BIN 16 (16.000 – 17.000 Å)
5502	CATS3D_17_NN	CATS3D Negative-Negative BIN 17 (17.000 – 18.000 Å)
5503	CATS3D_18_NN	CATS3D Negative-Negative BIN 18 (18.000 – 19.000 Å)
5504	CATS3D_19_NN	CATS3D Negative-Negative BIN 19 (19.000 – 20.000 Å)
5505	CATS3D_00_NL	CATS3D Negative-Lipophilic BIN 00 (0.000 – 1.000 Å)
5506	CATS3D_01_NL	CATS3D Negative-Lipophilic BIN 01 (1.000 – 2.000 Å)
5507	CATS3D_02_NL	CATS3D Negative-Lipophilic BIN 02 (2.000 – 3.000 Å)
5508	CATS3D_03_NL	CATS3D Negative-Lipophilic BIN 03 (3.000 – 4.000 Å)
5509	CATS3D_04_NL	CATS3D Negative-Lipophilic BIN 04 (4.000 – 5.000 Å)
5510	CATS3D_05_NL	CATS3D Negative-Lipophilic BIN 05 (5.000 – 6.000 Å)
5511	CATS3D_06_NL	CATS3D Negative-Lipophilic BIN 06 (6.000 – 7.000 Å)
5512	CATS3D_07_NL	CATS3D Negative-Lipophilic BIN 07 (7.000 – 8.000 Å)
5513	CATS3D_08_NL	CATS3D Negative-Lipophilic BIN 08 (8.000 – 9.000 Å)
5514	CATS3D_09_NL	CATS3D Negative-Lipophilic BIN 09 (9.000 – 10.000 Å)
5515	CATS3D_10_NL	CATS3D Negative-Lipophilic BIN 10 (10.000 – 11.000 Å)
5516	CATS3D_11_NL	CATS3D Negative-Lipophilic BIN 11 (11.000 – 12.000 Å)
5517	CATS3D_12_NL	CATS3D Negative-Lipophilic BIN 12 (12.000 – 13.000 Å)
5518	CATS3D_13_NL	CATS3D Negative-Lipophilic BIN 13 (13.000 – 14.000 Å)
5519	CATS3D_14_NL	CATS3D Negative-Lipophilic BIN 14 (14.000 – 15.000 Å)
5520	CATS3D_15_NL	CATS3D Negative-Lipophilic BIN 15 (15.000 – 16.000 Å)
5521	CATS3D_16_NL	CATS3D Negative-Lipophilic BIN 16 (16.000 – 17.000 Å)
5522	CATS3D_17_NL	CATS3D Negative-Lipophilic BIN 17 (17.000 – 18.000 Å)
5523	CATS3D_18_NL	CATS3D Negative-Lipophilic BIN 18 (18.000 – 19.000 Å)
5524	CATS3D_19_NL	CATS3D Negative-Lipophilic BIN 19 (19.000 – 20.000 Å)
5525	CATS3D_00_LL	CATS3D Lipophilic-Lipophilic BIN 00 (0.000 – 1.000 Å)
5526	CATS3D_01_LL	CATS3D Lipophilic-Lipophilic BIN 01 (1.000 – 2.000 Å)
5527	CATS3D_02_LL	CATS3D Lipophilic-Lipophilic BIN 02 (2.000 – 3.000 Å)
5528	CATS3D_03_LL	CATS3D Lipophilic-Lipophilic BIN 03 (3.000 – 4.000 Å)
5529	CATS3D_04_LL	CATS3D Lipophilic-Lipophilic BIN 04 (4.000 – 5.000 Å)
5530	CATS3D_05_LL	CATS3D Lipophilic-Lipophilic BIN 05 (5.000 – 6.000 Å)
5531	CATS3D_06_LL	CATS3D Lipophilic-Lipophilic BIN 06 (6.000 – 7.000 Å)
5532	CATS3D_07_LL	CATS3D Lipophilic-Lipophilic BIN 07 (7.000 – 8.000 Å)
5533	CATS3D_08_LL	CATS3D Lipophilic-Lipophilic BIN 08 (8.000 – 9.000 Å)
5534	CATS3D_09_LL	CATS3D Lipophilic-Lipophilic BIN 09 (9.000 – 10.000 Å)
5535	CATS3D_10_LL	CATS3D Lipophilic-Lipophilic BIN 10 (10.000 – 11.000 Å)
5536	CATS3D_11_LL	CATS3D Lipophilic-Lipophilic BIN 11 (11.000 – 12.000 Å)
5537	CATS3D_12_LL	CATS3D Lipophilic-Lipophilic BIN 12 (12.000 – 13.000 Å)
5538	CATS3D_13_LL	CATS3D Lipophilic-Lipophilic BIN 13 (13.000 – 14.000 Å)
5539	CATS3D_14_LL	CATS3D Lipophilic-Lipophilic BIN 14 (14.000 – 15.000 Å)
5540	CATS3D_15_LL	CATS3D Lipophilic-Lipophilic BIN 15 (15.000 – 16.000 Å)

5541	CATS3D_16_LL	CATS3D Lipophilic-Lipophilic BIN 16 (16.000 – 17.000 Å)
5542	CATS3D_17_LL	CATS3D Lipophilic-Lipophilic BIN 17 (17.000 – 18.000 Å)
5543	CATS3D_18_LL	CATS3D Lipophilic-Lipophilic BIN 18 (18.000 – 19.000 Å)
5544	CATS3D_19_LL	CATS3D Lipophilic-Lipophilic BIN 19 (19.000 – 20.000 Å)

31. WHALES descriptors

No.	Name	Description
5545	WHALES00_Rem	WHALES Remoteness (Rem) (percentile 00)
5546	WHALES10_Rem	WHALES Remoteness (Rem) (percentile 10)
5547	WHALES20_Rem	WHALES Remoteness (Rem) (percentile 20)
5548	WHALES30_Rem	WHALES Remoteness (Rem) (percentile 30)
5549	WHALES40_Rem	WHALES Remoteness (Rem) (percentile 40)
5550	WHALES50_Rem	WHALES Remoteness (Rem) (percentile 50)
5551	WHALES60_Rem	WHALES Remoteness (Rem) (percentile 60)
5552	WHALES70_Rem	WHALES Remoteness (Rem) (percentile 70)
5553	WHALES80_Rem	WHALES Remoteness (Rem) (percentile 80)
5554	WHALES90_Rem	WHALES Remoteness (Rem) (percentile 90)
5555	WHALES100_Rem	WHALES Remoteness (Rem) (percentile 100)
5556	WHALES00_Isol	WHALES Isolation degree (Isol) (percentile 00)
5557	WHALES10_Isol	WHALES Isolation degree (Isol) (percentile 10)
5558	WHALES20_Isol	WHALES Isolation degree (Isol) (percentile 20)
5559	WHALES30_Isol	WHALES Isolation degree (Isol) (percentile 30)
5560	WHALES40_Isol	WHALES Isolation degree (Isol) (percentile 40)
5561	WHALES50_Isol	WHALES Isolation degree (Isol) (percentile 50)
5562	WHALES60_Isol	WHALES Isolation degree (Isol) (percentile 60)
5563	WHALES70_Isol	WHALES Isolation degree (Isol) (percentile 70)
5564	WHALES80_Isol	WHALES Isolation degree (Isol) (percentile 80)
5565	WHALES90_Isol	WHALES Isolation degree (Isol) (percentile 90)
5566	WHALES100_Isol	WHALES Isolation degree (Isol) (percentile 100)
5567	WHALES00_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 00)
5568	WHALES10_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 10)
5569	WHALES20_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 20)
5570	WHALES30_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 30)
5571	WHALES40_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 40)
5572	WHALES50_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 50)
5573	WHALES60_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 60)
5574	WHALES70_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 70)
5575	WHALES80_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 80)
5576	WHALES90_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 90)
5577	WHALES100_IR	WHALES Isolation-Remoteness ratio (IR) (percentile 100)

32. MDE descriptors

No.	Name	Description

5578	MDEC-11	molecular distance edge between all primary carbons
5579	MDEC-12	molecular distance edge between all primary and secondary carbons
5580	MDEC-13	molecular distance edge between all primary and tertiary carbons
5581	MDEC-14	molecular distance edge between all primary and quaternary carbons
5582	MDEC-22	molecular distance edge between all secondary carbons
5583	MDEC-23	molecular distance edge between all secondary and tertiary carbons
5584	MDEC-24	molecular distance edge between all secondary and quaternary carbons
5585	MDEC-33	molecular distance edge between all tertiary carbons
5586	MDEC-34	molecular distance edge between all tertiary and quaternary carbons
5587	MDEC-44	molecular distance edge between all quaternary carbons
5588	MDEO-11	molecular distance edge between all primary oxygens
5589	MDEO-12	molecular distance edge between all primary and secondary oxygens
5590	MDEO-22	molecular distance edge between all secondary oxygens
5591	MDEN-11	molecular distance edge between all primary nitrogens
5592	MDEN-12	molecular distance edge between all primary and secondary nitrogens
5593	MDEN-13	molecular distance edge between all primary and tertiary niroqens
5594	MDEN-22	molecular distance edge between all secondary nitroqens
5595	MDEN-23	molecular distance edge between all secondary and tertiary nitrogens
5596	MDEN-33	molecular distance edge between all tertiary nitrogens

33. Chirality descriptors

No.	Name	Description
5597	ChiralCenter	number of chiral centres
5598	ringChiralCenter	number of chiral centres that are also ring atoms
5599	meanDistFromCC	mean pairwise distance considering all paths starting at the chiral centre
5600	maxDistfromCC	longest path starting from the chiral centre
5601	nLevel1	number of neighbouring atoms of the chiral centre (level 1)
5602	nLevel2	number of neighbouring atoms of the chiral centre (level 2)
5603	nLevel3	number of neighbouring atoms of the chiral centre (level 3)
5604	nLevel4	number of neighbouring atoms of the chiral centre (level 4)
5605	nLevel5	number of neighbouring atoms of the chiral centre (level 5)
5606	nLevel6	number of neighbouring atoms of the chiral centre (level 6)
5607	nLevel7	number of neighbouring atoms of the chiral centre (level 7)
5608	nLevel8	number of neighbouring atoms of the chiral centre (level 8)
5609	nLevel9	number of neighbouring atoms of the chiral centre (level 9)
5610	nLevel10	number of neighbouring atoms of the chiral centre (level 10)
5611	phLevel1	number of neighbouring N/O atoms of the chiral centre (level 1)
5612	phLevel2	number of neighbouring N/O atoms of the chiral centre (level 2)
5613	phLevel3	number of neighbouring N/O atoms of the chiral centre (level 3)
5614	arLevel1	number of neighbouring aromatic atoms of the chiral centre (level 1)
5615	arLevel2	number of neighbouring aromatic atoms of the chiral centre (level 2)
5616	arLevel3	number of neighbouring aromatic atoms of the chiral centre (level 3)

5617	s1_size	number of heavy atoms of the substituent 1 normalized by the atoms shared
5618	s2_size	number of heavy atoms of the substituent 2 normalized by the atoms shared
5619	s3_size	number of heavy atoms of the substituent 3 normalized by the atoms shared
5620	s4_size	number of heavy atoms of the substituent 4 normalized by the atoms shared
5621	s1_relSize	number of heavy atoms of the substituent 1 normalized by the heavy atoms
5622	s2_relSize	number of heavy atoms of the substituent 2 normalized by the heavy atoms
5623	s3_relSize	number of heavy atoms of the substituent 3 normalized by the heavy atoms
5624	s4_relSize	number of heavy atoms of the substituent 4 normalized by the heavy atoms
5625	s1_phSize	number of N/O atoms of the substituent 1 normalized by the N/O atoms shared
5626	s2_phSize	number of N/O atoms of the substituent 2 normalized by the N/O atoms shared
5627	s3_phSize	number of N/O atoms of the substituent 3 normalized by the N/O atoms shared
5628	s4_phSize	number of N/O atoms of the substituent 4 normalized by the N/O atoms shared
5629	s1_phRelSize	s1_phSize normalized by the heavy atoms
5630	s2_phRelSize	s2_phSize normalized by the heavy atoms
5631	s3_phRelSize	s3_phSize normalized by the heavy atoms
5632	s4_phRelSize	s4_phSize normalized by the heavy atoms
5633	s1_phRelSize_2	s1_phSize normalized by s1_size
5634	s2_phRelSize_2	s2_phSize normalized by s2_size
5635	s3_phRelSize_2	s3_phSize normalized by s3_size
5636	s4_phRelSize_2	s4_phSize normalized by s4_size
5637	s1_pathLength	maximum path length of the substituent 1
5638	s2_pathLength	maximum path length of the substituent 2
5639	s3_pathLength	maximum path length of the substituent 3
5640	s4_pathLength	maximum path length of the substituent 4
5641	s1_relPathLength	maximum path length of the substituent 1 normed by the heavy atoms
5642	s2_relPathLength	maximum path length of the substituent 2 normed by the heavy atoms
5643	s3_relPathLength	maximum path length of the substituent 3 normed by the heavy atoms
5644	s4_relPathLength	maximum path length of the substituent 4 normed by the heavy atoms
5645	s1_relPathLength_2	maximum path length of the substituent 1 normed by s1_size
5646	s2_relPathLength_2	maximum path length of the substituent 2 normed by s2_size
5647	s3_relPathLength_2	maximum path length of the substituent 3 normed by s3_size
5648	s4_relPathLength_2	maximum path length of the substituent 4 normed by s4_size
5649	s1_numSharedNeighbors	number of shared neighbours in substituent 1 with other substituents
5650	s2_numSharedNeighbors	number of shared neighbours in substituent 2 with other substituents
5651	s3_numSharedNeighbors	number of shared neighbours in substituent 3 with other substituents
5652	s4_numSharedNeighbors	number of shared neighbours in substituent 4 with other substituents
5653	s1_numRotBonds	number of rotatable bonds of the substituent 1
5654	s2_numRotBonds	number of rotatable bonds of the substituent 2
5655	s3_numRotBonds	number of rotatable bonds of the substituent 3
5656	s4_numRotBonds	number of rotatable bonds of the substituent 4
5657	s1_numAroBonds	number of aromatic bonds of the substituent 1
5658	s2_numAroBonds	number of aromatic bonds of the substituent 2

5659	s3_numAroBonds	number of aromatic bonds of the substituent 3
5660	s4_numAroBonds	number of aromatic bonds of the substituent 4
5661	s34_size	sum of s3_size and s4_size
5662	s34_relSize	sum of s3_relSize and s4_relSize
5663	s34_phSize	sum of s3_phSize and s4_phSize
5664	s34_phRelSize	sum of s3_phRelSize and s4_phRelSize
5665	chiralMoment	similar to the moment of inertia, but centred at the chiral centre
5666	chiralPhMoment	similar to chiralMoment, but only taking the N/O atoms into account