

No.	Rel.No.	Symbol	Definition	Class
1	1	MW	molecular weight	constitutional descriptors
2	2	AMW	average molecular weight	constitutional descriptors
3	3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)	constitutional descriptors
4	4	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)	constitutional descriptors
5	5	Sp	sum of atomic polarizabilities (scaled on Carbon atom)	constitutional descriptors
6	6	Ss	sum of Kier-Hall electrotopological states	constitutional descriptors
7	7	Mv	mean atomic van der Waals volume (scaled on Carbon atom)	constitutional descriptors
8	8	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)	constitutional descriptors
9	9	Mp	mean atomic polarizability (scaled on Carbon atom)	constitutional descriptors
10	10	Ms	mean electrotopological state	constitutional descriptors
11	11	nAT	number of atoms	constitutional descriptors
12	12	nSK	number of non-H atoms	constitutional descriptors
13	13	nBT	number of bonds	constitutional descriptors
14	14	nBO	number of non-H bonds	constitutional descriptors
15	15	nBM	number of multiple bonds	constitutional descriptors
16	16	SCBO	sum of conventional bond orders (H-depleted)	constitutional descriptors
17	17	ARR	aromatic ratio	constitutional descriptors

18	18	nCIC	number of rings	constitutional descriptors
19	19	nCIR	number of circuits	constitutional descriptors
20	20	RBN	number of rotatable bonds	constitutional descriptors
21	21	RBF	rotatable bond fraction	constitutional descriptors
22	22	nDB	number of double bonds	constitutional descriptors
23	23	nTB	number of triple bonds	constitutional descriptors
24	24	nAB	number of aromatic bonds	constitutional descriptors
25	25	nH	number of Hydrogen atoms	constitutional descriptors
26	26	nC	number of Carbon atoms	constitutional descriptors
27	27	nN	number of Nitrogen atoms	constitutional descriptors
28	28	nO	number of Oxygen atoms	constitutional descriptors
29	29	nP	number of Phosphorous atoms	constitutional descriptors
30	30	nS	number of Sulfur atoms	constitutional descriptors
31	31	nF	number of Fluorine atoms	constitutional descriptors
32	32	nCL	number of Chlorine atoms	constitutional descriptors
33	33	nBR	number of Bromine atoms	constitutional descriptors
34	34	nI	number of Iodine atoms	constitutional descriptors
35	35	nB	number of Boron atoms	constitutional descriptors

36	36	nHM	number of heavy atoms	constitutional descriptors
37	37	nX	number of halogen atoms	constitutional descriptors
38	38	nR03	number of 3-membered rings	constitutional descriptors
39	39	nR04	number of 4-membered rings	constitutional descriptors
40	40	nR05	number of 5-membered rings	constitutional descriptors
41	41	nR06	number of 6-membered rings	constitutional descriptors
42	42	nR07	number of 7-membered rings	constitutional descriptors
43	43	nR08	number of 8-membered rings	constitutional descriptors
44	44	nR09	number of 9-membered rings	constitutional descriptors
45	45	nR10	number of 10-membered rings	constitutional descriptors
46	46	nR11	number of 11-membered rings	constitutional descriptors
47	47	nR12	number of 12-membered rings	constitutional descriptors
48	48	nBnz	number of benzene-like rings	constitutional descriptors
49	1	ZM1	first Zagreb index M1	topological descriptors
50	2	ZM1V	first Zagreb index by valence vertex degrees	topological descriptors
51	3	ZM2	second Zagreb index M2	topological descriptors
52	4	ZM2V	second Zagreb index by valence vertex degrees	topological descriptors
53	5	Qindex	Quadratic index	topological descriptors

54	6	SNar	Narumi simple topological index (log)	topological descriptors
55	7	HNar	Narumi harmonic topological index	topological descriptors
56	8	GNar	Narumi geometric topological index	topological descriptors
57	9	Xt	Total structure connectivity index	topological descriptors
58	10	Dz	Pogliani index	topological descriptors
59	11	Ram	ramification index	topological descriptors
60	12	Pol	polarity number	topological descriptors
61	13	LPRS	log of product of row sums (PRS)	topological descriptors
62	14	VDA	average vertex distance degree	topological descriptors
63	15	MSD	mean square distance index (Balaban)	topological descriptors
64	16	SMTI	Schultz Molecular Topological Index (MTI)	topological descriptors
65	17	SMTIV	Schultz MTI by valence vertex degrees	topological descriptors
66	18	GMTI	Gutman Molecular Topological Index	topological descriptors
67	19	GMTIV	Gutman MTI by valence vertex degrees	topological descriptors
68	20	Xu	Xu index	topological descriptors
69	21	SPI	superpendentic index	topological descriptors
70	22	W	Wiener W index	topological descriptors
71	23	WA	mean Wiener index	topological descriptors

72	24	Har	Harary H index	topological descriptors
73	25	Har2	square reciprocal distance sum index	topological descriptors
74	26	QW	quasi-Wiener index (Kirchhoff number)	topological descriptors
75	27	TI1	first Mohar index TI1	topological descriptors
76	28	TI2	second Mohar index TI2	topological descriptors
77	29	STN	spanning tree number (log)	topological descriptors
78	30	HyDp	hyper-distance-path index	topological descriptors
79	31	RHyDp	reciprocal hyper-distance-path index	topological descriptors
80	32	w	detour index	topological descriptors
81	33	ww	hyper-detour index	topological descriptors
82	34	Rww	reciprocal hyper-detour index	topological descriptors
83	35	D/D	distance/detour index	topological descriptors
84	36	Wap	all-path Wiener index	topological descriptors
85	37	WhetZ	Wiener-type index from Z weighted distance matrix (Barysz matrix)	topological descriptors
86	38	Whetm	Wiener-type index from mass weighted distance matrix	topological descriptors
87	39	Whetv	Wiener-type index from van der Waals weighted distance matrix	topological descriptors
88	40	Whete	Wiener-type index from electronegativity weighted distance matrix	topological descriptors
89	41	Whetp	Wiener-type index from polarizability weighted distance matrix	topological descriptors

90	42	J	Balaban distance connectivity index	topological descriptors
91	43	JhetZ	Balaban-type index from Z weighted distance matrix (Barysz matrix)	topological descriptors
92	44	Jhetm	Balaban-type index from mass weighted distance matrix	topological descriptors
93	45	Jhetv	Balaban-type index from van der Waals weighted distance matrix	topological descriptors
94	46	Jhete	Balaban-type index from electronegativity weighted distance matrix	topological descriptors
95	47	Jhetp	Balaban-type index from polarizability weighted distance matrix	topological descriptors
96	48	MAXDN	maximal electrotopological negative variation	topological descriptors
97	49	MAXDP	maximal electrotopological positive variation	topological descriptors
98	50	DELS	molecular electrotopological variation	topological descriptors
99	51	TIE	E-state topological parameter	topological descriptors
100	52	S0K	Kier symmetry index	topological descriptors
101	53	S1K	1-path Kier alpha-modified shape index	topological descriptors
102	54	S2K	2-path Kier alpha-modified shape index	topological descriptors
103	55	S3K	3-path Kier alpha-modified shape index	topological descriptors
104	56	PHI	Kier flexibility index	topological descriptors
105	57	BLI	Kier benzene-likeliness index	topological descriptors
106	58	PW2	path/walk 2 - Randic shape index	topological descriptors
107	59	PW3	path/walk 3 - Randic shape index	topological descriptors

108	60	PW4	path/walk 4 - Randic shape index	topological descriptors
109	61	PW5	path/walk 5 - Randic shape index	topological descriptors
110	62	PJI2	2D Petitjean shape index	topological descriptors
111	63	CSI	eccentric connectivity index	topological descriptors
112	64	ECC	eccentricity	topological descriptors
113	65	AECC	average eccentricity	topological descriptors
114	66	DECC	eccentric	topological descriptors
115	67	MDDD	mean distance degree deviation	topological descriptors
116	68	UNIP	unipolarity	topological descriptors
117	69	CENT	centralization	topological descriptors
118	70	VAR	variation	topological descriptors
119	71	BAC	Balaban centric index	topological descriptors
120	72	Lop	Lopping centric index	topological descriptors
121	73	ICR	radial centric information index	topological descriptors
122	74	D/Dr03	distance/detour ring index of order 3	topological descriptors
123	75	D/Dr04	distance/detour ring index of order 4	topological descriptors
124	76	D/Dr05	distance/detour ring index of order 5	topological descriptors
125	77	D/Dr06	distance/detour ring index of order 6	topological descriptors

126	78	D/Dr07 distance/detour ring index of order 7	topological descriptors
127	79	D/Dr08 distance/detour ring index of order 8	topological descriptors
128	80	D/Dr09 distance/detour ring index of order 9	topological descriptors
129	81	D/Dr10 distance/detour ring index of order 10	topological descriptors
130	82	D/Dr11 distance/detour ring index of order 11	topological descriptors
131	83	D/Dr12 distance/detour ring index of order 12	topological descriptors
132	84	T(N..N) sum of topological distances between N..N	topological descriptors
133	85	T(N..O) sum of topological distances between N..O	topological descriptors
134	86	T(N..S) sum of topological distances between N..S	topological descriptors
135	87	T(N..P) sum of topological distances between N..P	topological descriptors
136	88	T(N..F) sum of topological distances between N..F	topological descriptors
137	89	T(N..Cl) sum of topological distances between N..Cl	topological descriptors
138	90	T(N..Br) sum of topological distances between N..Br	topological descriptors
139	91	T(N..I) sum of topological distances between N..I	topological descriptors
140	92	T(O..O) sum of topological distances between O..O	topological descriptors
141	93	T(O..S) sum of topological distances between O..S	topological descriptors
142	94	T(O..P) sum of topological distances between O..P	topological descriptors
143	95	T(O..F) sum of topological distances between O..F	topological descriptors

144	96	T(O..Cl) sum of topological distances between O..Cl	topological descriptors
145	97	T(O..Br) sum of topological distances between O..Br	topological descriptors
146	98	T(O..I) sum of topological distances between O..I	topological descriptors
147	99	T(S..S) sum of topological distances between S..S	topological descriptors
148	100	T(S..P) sum of topological distances between S..P	topological descriptors
149	101	T(S..F) sum of topological distances between S..F	topological descriptors
150	102	T(S..Cl) sum of topological distances between S..Cl	topological descriptors
151	103	T(S..Br) sum of topological distances between S..Br	topological descriptors
152	104	T(S..I) sum of topological distances between S..I	topological descriptors
153	105	T(P..P) sum of topological distances between P..P	topological descriptors
154	106	T(P..F) sum of topological distances between P..F	topological descriptors
155	107	T(P..Cl) sum of topological distances between P..Cl	topological descriptors
156	108	T(P..Br) sum of topological distances between P..Br	topological descriptors
157	109	T(P..I) sum of topological distances between P..I	topological descriptors
158	110	T(F..F) sum of topological distances between F..F	topological descriptors
159	111	T(F..Cl) sum of topological distances between F..Cl	topological descriptors
160	112	T(F..Br) sum of topological distances between F..Br	topological descriptors
161	113	T(F..I) sum of topological distances between F..I	topological descriptors

162	114	T(Cl..Cl)	sum of topological distances between Cl..Cl	topological descriptors	
163	115	T(Cl..Br)	sum of topological distances between Cl..Br	topological descriptors	
164	116	T(Cl..I)	sum of topological distances between Cl..I	topological descriptors	
165	117	T(Br..Br)	sum of topological distances between Br..Br	topological descriptors	
166	118	T(Br..I)	sum of topological distances between Br..I	topological descriptors	
167	119	T(I..I)	sum of topological distances between I..I	topological descriptors	
168	1	MWC01	molecular walk count of order 01 (number of non-H bonds, nBO)		walk and path counts
169	2	MWC02	molecular walk count of order 02	walk and path counts	
170	3	MWC03	molecular walk count of order 03	walk and path counts	
171	4	MWC04	molecular walk count of order 04	walk and path counts	
172	5	MWC05	molecular walk count of order 05	walk and path counts	
173	6	MWC06	molecular walk count of order 06	walk and path counts	
174	7	MWC07	molecular walk count of order 07	walk and path counts	
175	8	MWC08	molecular walk count of order 08	walk and path counts	
176	9	MWC09	molecular walk count of order 09	walk and path counts	
177	10	MWC10	molecular walk count of order 10	walk and path counts	
178	11	TWC	total walk count	walk and path counts	
179	12	SRW01	self-returning walk count of order 01 (number of non-H atoms, nSK)		walk and path counts

180	13	SRW02 self-returning walk count of order 02 (twice the number of non-H bonds)	walk and path counts
181	14	SRW03 self-returning walk count of order 03	walk and path counts
182	15	SRW04 self-returning walk count of order 04	walk and path counts
183	16	SRW05 self-returning walk count of order 05	walk and path counts
184	17	SRW06 self-returning walk count of order 06	walk and path counts
185	18	SRW07 self-returning walk count of order 07	walk and path counts
186	19	SRW08 self-returning walk count of order 08	walk and path counts
187	20	SRW09 self-returning walk count of order 09	walk and path counts
188	21	SRW10 self-returning walk count of order 10	walk and path counts
189	22	MPC01 molecular path count of order 01 (number of non-H bonds, nBO)	walk and path counts
190	23	MPC02 molecular path count of order 02 (Gordon-Scantlebury index)	walk and path counts
191	24	MPC03 molecular path count of order 03	walk and path counts
192	25	MPC04 molecular path count of order 04	walk and path counts
193	26	MPC05 molecular path count of order 05	walk and path counts
194	27	MPC06 molecular path count of order 06	walk and path counts
195	28	MPC07 molecular path count of order 07	walk and path counts
196	29	MPC08 molecular path count of order 08	walk and path counts
197	30	MPC09 molecular path count of order 09	walk and path counts

198	31	MPC10	molecular path count of order 10	walk and path counts
199	32	piPC01	molecular multiple path count of order 01 (sum of conventional bond orders, SCBO)	walk and path counts
200	33	piPC02	molecular multiple path count of order 02	walk and path counts
201	34	piPC03	molecular multiple path count of order 03	walk and path counts
202	35	piPC04	molecular multiple path count of order 04	walk and path counts
203	36	piPC05	molecular multiple path count of order 05	walk and path counts
204	37	piPC06	molecular multiple path count of order 06	walk and path counts
205	38	piPC07	molecular multiple path count of order 07	walk and path counts
206	39	piPC08	molecular multiple path count of order 08	walk and path counts
207	40	piPC09	molecular multiple path count of order 09	walk and path counts
208	41	piPC10	molecular multiple path count of order 10	walk and path counts
209	42	TPC	total path count	walk and path counts
210	43	piID	conventional bond-order ID number	walk and path counts
211	44	PCR	ratio of multiple path count over path count	walk and path counts
212	45	PCD	difference between multiple path count and path count	walk and path counts
213	46	CID	Randic ID number	walk and path counts
214	47	BID	Balaban ID number	walk and path counts
215	1	X0	connectivity index chi-0	connectivity indices

216	2	X1	connectivity index chi-1 (Randic connectivity index)	connectivity indices
217	3	X2	connectivity index chi-2	connectivity indices
218	4	X3	connectivity index chi-3	connectivity indices
219	5	X4	connectivity index chi-4	connectivity indices
220	6	X5	connectivity index chi-5	connectivity indices
221	7	X0A	average connectivity index chi-0	connectivity indices
222	8	X1A	average connectivity index chi-1	connectivity indices
223	9	X2A	average connectivity index chi-2	connectivity indices
224	10	X3A	average connectivity index chi-3	connectivity indices
225	11	X4A	average connectivity index chi-4	connectivity indices
226	12	X5A	average connectivity index chi-5	connectivity indices
227	13	X0v	valence connectivity index chi-0	connectivity indices
228	14	X1v	valence connectivity index chi-1	connectivity indices
229	15	X2v	valence connectivity index chi-2	connectivity indices
230	16	X3v	valence connectivity index chi-3	connectivity indices
231	17	X4v	valence connectivity index chi-4	connectivity indices
232	18	X5v	valence connectivity index chi-5	connectivity indices
233	19	X0Av	average valence connectivity index chi-0	connectivity indices

234	20	X1Av	average valence connectivity index chi-1	connectivity indices
235	21	X2Av	average valence connectivity index chi-2	connectivity indices
236	22	X3Av	average valence connectivity index chi-3	connectivity indices
237	23	X4Av	average valence connectivity index chi-4	connectivity indices
238	24	X5Av	average valence connectivity index chi-5	connectivity indices
239	25	X0sol	solvation connectivity index chi-0	connectivity indices
240	26	X1sol	solvation connectivity index chi-1	connectivity indices
241	27	X2sol	solvation connectivity index chi-2	connectivity indices
242	28	X3sol	solvation connectivity index chi-3	connectivity indices
243	29	X4sol	solvation connectivity index chi-4	connectivity indices
244	30	X5sol	solvation connectivity index chi-5	connectivity indices
245	31	XMOD	modified Randic connectivity index	connectivity indices
246	32	RDCHI	reciprocal distance Randic-type index	connectivity indices
247	33	RDSQ	reciprocal distance squared Randic-type index	connectivity indices
248	1	ISIZ	information index on molecular size	information indices
249	2	IAC	total information index of atomic composition	information indices
250	3	AAC	mean information index on atomic composition	information indices
251	4	IDE	mean information content on the distance equality	information indices

252	5	IDM	mean information content on the distance magnitude	information indices
253	6	IDDE	mean information content on the distance degree equality	information indices
254	7	IDDM	mean information content on the distance degree magnitude	information indices
255	8	IDET	total information content on the distance equality	information indices
256	9	IDMT	total information content on the distance magnitude	information indices
257	10	IVDE	mean information content on the vertex degree equality	information indices
258	11	IVDM	mean information content on the vertex degree magnitude	information indices
259	12	HVcpx	graph vertex complexity index	information indices
260	13	HDcpx	graph distance complexity index (log)	information indices
261	14	Uindex	Balaban U index	information indices
262	15	Vindex	Balaban V index	information indices
263	16	Xindex	Balaban X index	information indices
264	17	Yindex	Balaban Y index	information indices
265	18	ICO	information content index (neighborhood symmetry of 0-order)	information indices
266	19	TICO	total information content index (neighborhood symmetry of 0-order)	information indices
267	20	SICO	structural information content (neighborhood symmetry of 0-order)	information indices
268	21	CICO	complementary information content (neighborhood symmetry of 0-order)	information indices
269	22	BICO	bond information content (neighborhood symmetry of 0-order)	information indices

270	23	IC1	information content index (neighborhood symmetry of 1-order)	information indices
271	24	TIC1	total information content index (neighborhood symmetry of 1-order)	information indices
272	25	SIC1	structural information content (neighborhood symmetry of 1-order)	information indices
273	26	CIC1	complementary information content (neighborhood symmetry of 1-order)	information indices
274	27	BIC1	bond information content (neighborhood symmetry of 1-order)	information indices
275	28	IC2	information content index (neighborhood symmetry of 2-order)	information indices
276	29	TIC2	total information content index (neighborhood symmetry of 2-order)	information indices
277	30	SIC2	structural information content (neighborhood symmetry of 2-order)	information indices
278	31	CIC2	complementary information content (neighborhood symmetry of 2-order)	information indices
279	32	BIC2	bond information content (neighborhood symmetry of 2-order)	information indices
280	33	IC3	information content index (neighborhood symmetry of 3-order)	information indices
281	34	TIC3	total information content index (neighborhood symmetry of 3-order)	information indices
282	35	SIC3	structural information content (neighborhood symmetry of 3-order)	information indices
283	36	CIC3	complementary information content (neighborhood symmetry of 3-order)	information indices
284	37	BIC3	bond information content (neighborhood symmetry of 3-order)	information indices
285	38	IC4	information content index (neighborhood symmetry of 4-order)	information indices
286	39	TIC4	total information content index (neighborhood symmetry of 4-order)	information indices
287	40	SIC4	structural information content (neighborhood symmetry of 4-order)	information indices

288	41	CIC4	complementary information content (neighborhood symmetry of 4-order)	information indices
289	42	BIC4	bond information content (neighborhood symmetry of 4-order)	information indices
290	43	IC5	information content index (neighborhood symmetry of 5-order)	information indices
291	44	TIC5	total information content index (neighborhood symmetry of 5-order)	information indices
292	45	SIC5	structural information content (neighborhood symmetry of 5-order)	information indices
293	46	CIC5	complementary information content (neighborhood symmetry of 5-order)	information indices
294	47	BIC5	bond information content (neighborhood symmetry of 5-order)	information indices
295	1	ATS1m	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic masses	2D autocorrelations
296	2	ATS2m	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic masses	2D autocorrelations
297	3	ATS3m	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic masses	2D autocorrelations
298	4	ATS4m	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic masses	2D autocorrelations
299	5	ATS5m	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic masses	2D autocorrelations
300	6	ATS6m	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic masses	2D autocorrelations
301	7	ATS7m	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic masses	2D autocorrelations
302	8	ATS8m	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic masses	2D autocorrelations
303	9	ATS1v	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
304	10	ATS2v	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
305	11	ATS3v	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations

306	12	ATS4v	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
307	13	ATS5v	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
308	14	ATS6v	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
309	15	ATS7v	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations
310	16	ATS8v	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
311	17	ATS1e	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
312	18	ATS2e	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
313	19	ATS3e	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations
314	20	ATS4e	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
315	21	ATS5e	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
316	22	ATS6e	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations
317	23	ATS7e	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
318	24	ATS8e	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
319	25	ATS1p	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
320	26	ATS2p	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
321	27	ATS3p	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
322	28	ATS4p	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
323	29	ATS5p	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic polarizabilities	2D autocorrelations

324	30	ATS6p	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
325	31	ATS7p	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
326	32	ATS8p	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
327	33	MATS1m	Moran autocorrelation - lag 1 / weighted by atomic masses	2D autocorrelations
328	34	MATS2m	Moran autocorrelation - lag 2 / weighted by atomic masses	2D autocorrelations
329	35	MATS3m	Moran autocorrelation - lag 3 / weighted by atomic masses	2D autocorrelations
330	36	MATS4m	Moran autocorrelation - lag 4 / weighted by atomic masses	2D autocorrelations
331	37	MATS5m	Moran autocorrelation - lag 5 / weighted by atomic masses	2D autocorrelations
332	38	MATS6m	Moran autocorrelation - lag 6 / weighted by atomic masses	2D autocorrelations
333	39	MATS7m	Moran autocorrelation - lag 7 / weighted by atomic masses	2D autocorrelations
334	40	MATS8m	Moran autocorrelation - lag 8 / weighted by atomic masses	2D autocorrelations
335	41	MATS1v	Moran autocorrelation - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
336	42	MATS2v	Moran autocorrelation - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
337	43	MATS3v	Moran autocorrelation - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations
338	44	MATS4v	Moran autocorrelation - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
339	45	MATS5v	Moran autocorrelation - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
340	46	MATS6v	Moran autocorrelation - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
341	47	MATS7v	Moran autocorrelation - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations

342	48	MATS8v	Moran autocorrelation - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
343	49	MATS1e	Moran autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
344	50	MATS2e	Moran autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
345	51	MATS3e	Moran autocorrelation - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations
346	52	MATS4e	Moran autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
347	53	MATS5e	Moran autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
348	54	MATS6e	Moran autocorrelation - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations
349	55	MATS7e	Moran autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
350	56	MATS8e	Moran autocorrelation - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
351	57	MATS1p	Moran autocorrelation - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
352	58	MATS2p	Moran autocorrelation - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
353	59	MATS3p	Moran autocorrelation - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
354	60	MATS4p	Moran autocorrelation - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
355	61	MATS5p	Moran autocorrelation - lag 5 / weighted by atomic polarizabilities	2D autocorrelations
356	62	MATS6p	Moran autocorrelation - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
357	63	MATS7p	Moran autocorrelation - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
358	64	MATS8p	Moran autocorrelation - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
359	65	GATS1m	Geary autocorrelation - lag 1 / weighted by atomic masses	2D autocorrelations

360	66	GATS2m	Geary autocorrelation - lag 2 / weighted by atomic masses	2D autocorrelations
361	67	GATS3m	Geary autocorrelation - lag 3 / weighted by atomic masses	2D autocorrelations
362	68	GATS4m	Geary autocorrelation - lag 4 / weighted by atomic masses	2D autocorrelations
363	69	GATS5m	Geary autocorrelation - lag 5 / weighted by atomic masses	2D autocorrelations
364	70	GATS6m	Geary autocorrelation - lag 6 / weighted by atomic masses	2D autocorrelations
365	71	GATS7m	Geary autocorrelation - lag 7 / weighted by atomic masses	2D autocorrelations
366	72	GATS8m	Geary autocorrelation - lag 8 / weighted by atomic masses	2D autocorrelations
367	73	GATS1v	Geary autocorrelation - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
368	74	GATS2v	Geary autocorrelation - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
369	75	GATS3v	Geary autocorrelation - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations
370	76	GATS4v	Geary autocorrelation - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
371	77	GATS5v	Geary autocorrelation - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
372	78	GATS6v	Geary autocorrelation - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
373	79	GATS7v	Geary autocorrelation - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations
374	80	GATS8v	Geary autocorrelation - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
375	81	GATS1e	Geary autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
376	82	GATS2e	Geary autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
377	83	GATS3e	Geary autocorrelation - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations

378	84	GATS4eGeary autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
379	85	GATS5eGeary autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
380	86	GATS6eGeary autocorrelation - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations
381	87	GATS7eGeary autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
382	88	GATS8eGeary autocorrelation - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
383	89	GATS1pGeary autocorrelation - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
384	90	GATS2pGeary autocorrelation - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
385	91	GATS3pGeary autocorrelation - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
386	92	GATS4pGeary autocorrelation - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
387	93	GATS5pGeary autocorrelation - lag 5 / weighted by atomic polarizabilities	2D autocorrelations
388	94	GATS6pGeary autocorrelation - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
389	95	GATS7pGeary autocorrelation - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
390	96	GATS8pGeary autocorrelation - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
391	1	EPS0 edge connectivity index of order 0	edge adjacency indices
392	2	EPS1 edge connectivity index of order 1	edge adjacency indices
393	3	EEig01xEigenvalue 01 from edge adj. matrix weighted by edge degrees	edge adjacency indices
394	4	EEig02xEigenvalue 02 from edge adj. matrix weighted by edge degrees	edge adjacency indices
395	5	EEig03xEigenvalue 03 from edge adj. matrix weighted by edge degrees	edge adjacency indices

396	6	EEig04xEigenvalue 04 from edge adj. matrix weighted by edge degrees edge adjacency indices
397	7	EEig05xEigenvalue 05 from edge adj. matrix weighted by edge degrees edge adjacency indices
398	8	EEig06xEigenvalue 06 from edge adj. matrix weighted by edge degrees edge adjacency indices
399	9	EEig07xEigenvalue 07 from edge adj. matrix weighted by edge degrees edge adjacency indices
400	10	EEig08xEigenvalue 08 from edge adj. matrix weighted by edge degrees edge adjacency indices
401	11	EEig09xEigenvalue 09 from edge adj. matrix weighted by edge degrees edge adjacency indices
402	12	EEig10xEigenvalue 10 from edge adj. matrix weighted by edge degrees edge adjacency indices
403	13	EEig11xEigenvalue 11 from edge adj. matrix weighted by edge degrees edge adjacency indices
404	14	EEig12xEigenvalue 12 from edge adj. matrix weighted by edge degrees edge adjacency indices
405	15	EEig13xEigenvalue 13 from edge adj. matrix weighted by edge degrees edge adjacency indices
406	16	EEig14xEigenvalue 14 from edge adj. matrix weighted by edge degrees edge adjacency indices
407	17	EEig15xEigenvalue 15 from edge adj. matrix weighted by edge degrees edge adjacency indices
408	18	EEig01dEigenvalue 01 from edge adj. matrix weighted by dipole moments edge adjacency indices
409	19	EEig02dEigenvalue 02 from edge adj. matrix weighted by dipole moments edge adjacency indices
410	20	EEig03dEigenvalue 03 from edge adj. matrix weighted by dipole moments edge adjacency indices
411	21	EEig04dEigenvalue 04 from edge adj. matrix weighted by dipole moments edge adjacency indices
412	22	EEig05dEigenvalue 05 from edge adj. matrix weighted by dipole moments edge adjacency indices
413	23	EEig06dEigenvalue 06 from edge adj. matrix weighted by dipole moments edge adjacency indices

414	24	EEig07dEigenvalue 07 from edge adj. matrix weighted by dipole moments	edge adjacency indices
415	25	EEig08dEigenvalue 08 from edge adj. matrix weighted by dipole moments	edge adjacency indices
416	26	EEig09dEigenvalue 09 from edge adj. matrix weighted by dipole moments	edge adjacency indices
417	27	EEig10dEigenvalue 10 from edge adj. matrix weighted by dipole moments	edge adjacency indices
418	28	EEig11dEigenvalue 11 from edge adj. matrix weighted by dipole moments	edge adjacency indices
419	29	EEig12dEigenvalue 12 from edge adj. matrix weighted by dipole moments	edge adjacency indices
420	30	EEig13dEigenvalue 13 from edge adj. matrix weighted by dipole moments	edge adjacency indices
421	31	EEig14dEigenvalue 14 from edge adj. matrix weighted by dipole moments	edge adjacency indices
422	32	EEig15dEigenvalue 15 from edge adj. matrix weighted by dipole moments	edge adjacency indices
423	33	EEig01r Eigenvalue 01 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
424	34	EEig02r Eigenvalue 02 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
425	35	EEig03r Eigenvalue 03 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
426	36	EEig04r Eigenvalue 04 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
427	37	EEig05r Eigenvalue 05 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
428	38	EEig06r Eigenvalue 06 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
429	39	EEig07r Eigenvalue 07 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
430	40	EEig08r Eigenvalue 08 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
431	41	EEig09r Eigenvalue 09 from edge adj. matrix weighted by resonance integrals	edge adjacency indices

432	42	EEig10r Eigenvalue 10 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
433	43	EEig11r Eigenvalue 11 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
434	44	EEig12r Eigenvalue 12 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
435	45	EEig13r Eigenvalue 13 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
436	46	EEig14r Eigenvalue 14 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
437	47	EEig15r Eigenvalue 15 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
438	48	ESpm01u Spectral moment 01 from edge adj. matrix	edge adjacency indices
439	49	ESpm02u Spectral moment 02 from edge adj. matrix	edge adjacency indices
440	50	ESpm03u Spectral moment 03 from edge adj. matrix	edge adjacency indices
441	51	ESpm04u Spectral moment 04 from edge adj. matrix	edge adjacency indices
442	52	ESpm05u Spectral moment 05 from edge adj. matrix	edge adjacency indices
443	53	ESpm06u Spectral moment 06 from edge adj. matrix	edge adjacency indices
444	54	ESpm07u Spectral moment 07 from edge adj. matrix	edge adjacency indices
445	55	ESpm08u Spectral moment 08 from edge adj. matrix	edge adjacency indices
446	56	ESpm09u Spectral moment 09 from edge adj. matrix	edge adjacency indices
447	57	ESpm10u Spectral moment 10 from edge adj. matrix	edge adjacency indices
448	58	ESpm11u Spectral moment 11 from edge adj. matrix	edge adjacency indices
449	59	ESpm12u Spectral moment 12 from edge adj. matrix	edge adjacency indices

450	60	ESpm13u	Spectral moment 13 from edge adj. matrix	edge adjacency indices
451	61	ESpm14u	Spectral moment 14 from edge adj. matrix	edge adjacency indices
452	62	ESpm15u	Spectral moment 15 from edge adj. matrix	edge adjacency indices
453	63	ESpm01x	Spectral moment 01 from edge adj. matrix weighted by edge degrees	edge adjacency indices
454	64	ESpm02x	Spectral moment 02 from edge adj. matrix weighted by edge degrees	edge adjacency indices
455	65	ESpm03x	Spectral moment 03 from edge adj. matrix weighted by edge degrees	edge adjacency indices
456	66	ESpm04x	Spectral moment 04 from edge adj. matrix weighted by edge degrees	edge adjacency indices
457	67	ESpm05x	Spectral moment 05 from edge adj. matrix weighted by edge degrees	edge adjacency indices
458	68	ESpm06x	Spectral moment 06 from edge adj. matrix weighted by edge degrees	edge adjacency indices
459	69	ESpm07x	Spectral moment 07 from edge adj. matrix weighted by edge degrees	edge adjacency indices
460	70	ESpm08x	Spectral moment 08 from edge adj. matrix weighted by edge degrees	edge adjacency indices
461	71	ESpm09x	Spectral moment 09 from edge adj. matrix weighted by edge degrees	edge adjacency indices
462	72	ESpm10x	Spectral moment 10 from edge adj. matrix weighted by edge degrees	edge adjacency indices
463	73	ESpm11x	Spectral moment 11 from edge adj. matrix weighted by edge degrees	edge adjacency indices
464	74	ESpm12x	Spectral moment 12 from edge adj. matrix weighted by edge degrees	edge adjacency indices
465	75	ESpm13x	Spectral moment 13 from edge adj. matrix weighted by edge degrees	edge adjacency indices
466	76	ESpm14x	Spectral moment 14 from edge adj. matrix weighted by edge degrees	edge adjacency indices
467	77	ESpm15x	Spectral moment 15 from edge adj. matrix weighted by edge degrees	edge adjacency indices

468	78	ESpm01d	Spectral moment 01 from edge adj. matrix weighted by dipole moments	edge adjacency indices
469	79	ESpm02d	Spectral moment 02 from edge adj. matrix weighted by dipole moments	edge adjacency indices
470	80	ESpm03d	Spectral moment 03 from edge adj. matrix weighted by dipole moments	edge adjacency indices
471	81	ESpm04d	Spectral moment 04 from edge adj. matrix weighted by dipole moments	edge adjacency indices
472	82	ESpm05d	Spectral moment 05 from edge adj. matrix weighted by dipole moments	edge adjacency indices
473	83	ESpm06d	Spectral moment 06 from edge adj. matrix weighted by dipole moments	edge adjacency indices
474	84	ESpm07d	Spectral moment 07 from edge adj. matrix weighted by dipole moments	edge adjacency indices
475	85	ESpm08d	Spectral moment 08 from edge adj. matrix weighted by dipole moments	edge adjacency indices
476	86	ESpm09d	Spectral moment 09 from edge adj. matrix weighted by dipole moments	edge adjacency indices
477	87	ESpm10d	Spectral moment 10 from edge adj. matrix weighted by dipole moments	edge adjacency indices
478	88	ESpm11d	Spectral moment 11 from edge adj. matrix weighted by dipole moments	edge adjacency indices
479	89	ESpm12d	Spectral moment 12 from edge adj. matrix weighted by dipole moments	edge adjacency indices
480	90	ESpm13d	Spectral moment 13 from edge adj. matrix weighted by dipole moments	edge adjacency indices
481	91	ESpm14d	Spectral moment 14 from edge adj. matrix weighted by dipole moments	edge adjacency indices
482	92	ESpm15d	Spectral moment 15 from edge adj. matrix weighted by dipole moments	edge adjacency indices
483	93	ESpm01r	Spectral moment 01 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
484	94	ESpm02r	Spectral moment 02 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
485	95	ESpm03r	Spectral moment 03 from edge adj. matrix weighted by resonance integrals	edge adjacency indices

486	96	ESpm04r	Spectral moment 04 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
487	97	ESpm05r	Spectral moment 05 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
488	98	ESpm06r	Spectral moment 06 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
489	99	ESpm07r	Spectral moment 07 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
490	100	ESpm08r	Spectral moment 08 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
491	101	ESpm09r	Spectral moment 09 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
492	102	ESpm10r	Spectral moment 10 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
493	103	ESpm11r	Spectral moment 11 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
494	104	ESpm12r	Spectral moment 12 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
495	105	ESpm13r	Spectral moment 13 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
496	106	ESpm14r	Spectral moment 14 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
497	107	ESpm15r	Spectral moment 15 from edge adj. matrix weighted by resonance integrals	edge adjacency indices
498	1	BEHm1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic masses	Burden eigenvalues
499	2	BEHm2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic masses	Burden eigenvalues
500	3	BEHm3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic masses	Burden eigenvalues
501	4	BEHm4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic masses	Burden eigenvalues
502	5	BEHm5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic masses	Burden eigenvalues
503	6	BEHm6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic masses	Burden eigenvalues

504	7	BEHm7 highest eigenvalue n. 7 of Burden matrix / weighted by atomic masses	Burden eigenvalues
505	8	BEHm8 highest eigenvalue n. 8 of Burden matrix / weighted by atomic masses	Burden eigenvalues
506	9	BELm1 lowest eigenvalue n. 1 of Burden matrix / weighted by atomic masses	Burden eigenvalues
507	10	BELm2 lowest eigenvalue n. 2 of Burden matrix / weighted by atomic masses	Burden eigenvalues
508	11	BELm3 lowest eigenvalue n. 3 of Burden matrix / weighted by atomic masses	Burden eigenvalues
509	12	BELm4 lowest eigenvalue n. 4 of Burden matrix / weighted by atomic masses	Burden eigenvalues
510	13	BELm5 lowest eigenvalue n. 5 of Burden matrix / weighted by atomic masses	Burden eigenvalues
511	14	BELm6 lowest eigenvalue n. 6 of Burden matrix / weighted by atomic masses	Burden eigenvalues
512	15	BELm7 lowest eigenvalue n. 7 of Burden matrix / weighted by atomic masses	Burden eigenvalues
513	16	BELm8 lowest eigenvalue n. 8 of Burden matrix / weighted by atomic masses	Burden eigenvalues
514	17	BEHv1 highest eigenvalue n. 1 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
515	18	BEHv2 highest eigenvalue n. 2 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
516	19	BEHv3 highest eigenvalue n. 3 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
517	20	BEHv4 highest eigenvalue n. 4 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
518	21	BEHv5 highest eigenvalue n. 5 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
519	22	BEHv6 highest eigenvalue n. 6 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
520	23	BEHv7 highest eigenvalue n. 7 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
521	24	BEHv8 highest eigenvalue n. 8 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues

522	25	BELv1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
523	26	BELv2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
524	27	BELv3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
525	28	BELv4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
526	29	BELv5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
527	30	BELv6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
528	31	BELv7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
529	32	BELv8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic van der Waals volumes	Burden eigenvalues
530	33	BEHe1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
531	34	BEHe2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
532	35	BEHe3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
533	36	BEHe4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
534	37	BEHe5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
535	38	BEHe6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
536	39	BEHe7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
537	40	BEHe8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
538	41	BELe1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
539	42	BELe2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues

540	43	BELe3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
541	44	BELe4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
542	45	BELe5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
543	46	BELe6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
544	47	BELe7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
545	48	BELe8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic Sanderson electronegativities	Burden eigenvalues
546	49	BEHp1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
547	50	BEHp2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
548	51	BEHp3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
549	52	BEHp4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
550	53	BEHp5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
551	54	BEHp6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
552	55	BEHp7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
553	56	BEHp8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
554	57	BELp1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
555	58	BELp2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
556	59	BELp3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
557	60	BELp4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues

558	61	BELp5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
559	62	BELp6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
560	63	BELp7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
561	64	BELp8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic polarizabilities	Burden eigenvalues
562	1	GGI1	topological charge index of order 1	topological charge indices
563	2	GGI2	topological charge index of order 2	topological charge indices
564	3	GGI3	topological charge index of order 3	topological charge indices
565	4	GGI4	topological charge index of order 4	topological charge indices
566	5	GGI5	topological charge index of order 5	topological charge indices
567	6	GGI6	topological charge index of order 6	topological charge indices
568	7	GGI7	topological charge index of order 7	topological charge indices
569	8	GGI8	topological charge index of order 8	topological charge indices
570	9	GGI9	topological charge index of order 9	topological charge indices
571	10	GGI10	topological charge index of order 10	topological charge indices
572	11	JGI1	mean topological charge index of order1	topological charge indices
573	12	JGI2	mean topological charge index of order2	topological charge indices
574	13	JGI3	mean topological charge index of order3	topological charge indices
575	14	JGI4	mean topological charge index of order4	topological charge indices

576	15	JGI5	mean topological charge index of order5	topological charge indices
577	16	JGI6	mean topological charge index of order6	topological charge indices
578	17	JGI7	mean topological charge index of order7	topological charge indices
579	18	JGI8	mean topological charge index of order8	topological charge indices
580	19	JGI9	mean topological charge index of order9	topological charge indices
581	20	JGI10	mean topological charge index of order10	topological charge indices
582	21	JGT	global topological charge index	topological charge indices
583	1	LP1	Lovasz-Pelikan index (leading eigenvalue)	eigenvalue-based indices
584	2	Eig1Z	Leading eigenvalue from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
585	3	Eig1m	Leading eigenvalue from mass weighted distance matrix	eigenvalue-based indices
586	4	Eig1v	Leading eigenvalue from van der Waals weighted distance matrix	eigenvalue-based indices
587	5	Eig1e	Leading eigenvalue from electronegativity weighted distance matrix	eigenvalue-based indices
588	6	Eig1p	Leading eigenvalue from polarizability weighted distance matrix	eigenvalue-based indices
589	7	SEigZ	Eigenvalue sum from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
590	8	SEigm	Eigenvalue sum from mass weighted distance matrix	eigenvalue-based indices
591	9	SEigv	Eigenvalue sum from van der Waals weighted distance matrix	eigenvalue-based indices
592	10	SEige	Eigenvalue sum from electronegativity weighted distance matrix	eigenvalue-based indices
593	11	SEigp	Eigenvalue sum from polarizability weighted distance matrix	eigenvalue-based indices

594	12	AEigZ	Absolute eigenvalue sum from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
595	13	AEigm	Absolute eigenvalue sum from mass weighted distance matrix	eigenvalue-based indices
596	14	AEigv	Absolute eigenvalue sum from van der Waals weighted distance matrix	eigenvalue-based indices
597	15	AEige	Absolute eigenvalue sum from electronegativity weighted distance matrix	eigenvalue-based indices
598	16	AEigp	Absolute eigenvalue sum from polarizability weighted distance matrix	eigenvalue-based indices
599	17	VEA1	eigenvector coefficient sum from adjacency matrix	eigenvalue-based indices
600	18	VEA2	average eigenvector coefficient sum from adjacency matrix	eigenvalue-based indices
601	19	VRA1	Randic-type eigenvector-based index from adjacency matrix	eigenvalue-based indices
602	20	VRA2	average Randic-type eigenvector-based index from adjacency matrix	eigenvalue-based indices
603	21	VED1	eigenvector coefficient sum from distance matrix	eigenvalue-based indices
604	22	VED2	average eigenvector coefficient sum from distance matrix	eigenvalue-based indices
605	23	VRD1	Randic-type eigenvector-based index from distance matrix	eigenvalue-based indices
606	24	VRD2	average Randic-type eigenvector-based index from distance matrix	eigenvalue-based indices
607	25	VEZ1	eigenvector coefficient sum from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
608	26	VEZ2	average eigenvector coefficient sum from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
609	27	VRZ1	Randic-type eigenvector-based index from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
610	28	VRZ2	average Randic-type eigenvector-based index from Z weighted distance matrix (Barysz matrix)	eigenvalue-based indices
611	29	VEm1	eigenvector coefficient sum from mass weighted distance matrix	eigenvalue-based indices

612	30	VEm2	average eigenvector coefficient sum from mass weighted distance matrix	eigenvalue-based indices
613	31	VRm1	Randic-type eigenvector-based index from mass weighted distance matrix	eigenvalue-based indices
614	32	VRm2	average Randic-type eigenvector-based index from mass weighted distance matrix	eigenvalue-based indices
615	33	VEv1	eigenvector coefficient sum from van der Waals weighted distance matrix	eigenvalue-based indices
616	34	VEv2	average eigenvector coefficient sum from van der Waals weighted distance matrix	eigenvalue-based indices
617	35	VRv1	Randic-type eigenvector-based index from van der Waals weighted distance matrix	eigenvalue-based indices
618	36	VRv2	average Randic-type eigenvector-based index from van der Waals weighted distance matrix	eigenvalue-based indices
619	37	VEe1	eigenvector coefficient sum from electronegativity weighted distance matrix	eigenvalue-based indices
620	38	VEe2	average eigenvector coefficient sum from electronegativity weighted distance matrix	eigenvalue-based indices
621	39	VRe1	Randic-type eigenvector-based index from electronegativity weighted distance matrix	eigenvalue-based indices
622	40	VRe2	average Randic-type eigenvector-based index from electronegativity weighted distance matrix	eigenvalue-based indices
623	41	VEp1	eigenvector coefficient sum from polarizability weighted distance matrix	eigenvalue-based indices
624	42	VEp2	average eigenvector coefficient sum from polarizability weighted distance matrix	eigenvalue-based indices
625	43	VRp1	Randic-type eigenvector-based index from polarizability weighted distance matrix	eigenvalue-based indices
626	44	VRp2	average Randic-type eigenvector-based index from polarizability weighted distance matrix	eigenvalue-based indices
627	1	DP01	molecular profile no. 01	Randic molecular profiles
628	2	DP02	molecular profile no. 02	Randic molecular profiles
629	3	DP03	molecular profile no. 03	Randic molecular profiles

630	4	DP04	molecular profile no. 04	Randic molecular profiles
631	5	DP05	molecular profile no. 05	Randic molecular profiles
632	6	DP06	molecular profile no. 06	Randic molecular profiles
633	7	DP07	molecular profile no. 07	Randic molecular profiles
634	8	DP08	molecular profile no. 08	Randic molecular profiles
635	9	DP09	molecular profile no. 09	Randic molecular profiles
636	10	DP10	molecular profile no. 10	Randic molecular profiles
637	11	DP11	molecular profile no. 11	Randic molecular profiles
638	12	DP12	molecular profile no. 12	Randic molecular profiles
639	13	DP13	molecular profile no. 13	Randic molecular profiles
640	14	DP14	molecular profile no. 14	Randic molecular profiles
641	15	DP15	molecular profile no. 15	Randic molecular profiles
642	16	DP16	molecular profile no. 16	Randic molecular profiles
643	17	DP17	molecular profile no. 17	Randic molecular profiles
644	18	DP18	molecular profile no. 18	Randic molecular profiles
645	19	DP19	molecular profile no. 19	Randic molecular profiles
646	20	DP20	molecular profile no. 20	Randic molecular profiles
647	21	SP01	shape profile no. 01	Randic molecular profiles

648	22	SP02	shape profile no. 02	Randic molecular profiles
649	23	SP03	shape profile no. 03	Randic molecular profiles
650	24	SP04	shape profile no. 04	Randic molecular profiles
651	25	SP05	shape profile no. 05	Randic molecular profiles
652	26	SP06	shape profile no. 06	Randic molecular profiles
653	27	SP07	shape profile no. 07	Randic molecular profiles
654	28	SP08	shape profile no. 08	Randic molecular profiles
655	29	SP09	shape profile no. 09	Randic molecular profiles
656	30	SP10	shape profile no. 10	Randic molecular profiles
657	31	SP11	shape profile no. 11	Randic molecular profiles
658	32	SP12	shape profile no. 12	Randic molecular profiles
659	33	SP13	shape profile no. 13	Randic molecular profiles
660	34	SP14	shape profile no. 14	Randic molecular profiles
661	35	SP15	shape profile no. 15	Randic molecular profiles
662	36	SP16	shape profile no. 16	Randic molecular profiles
663	37	SP17	shape profile no. 17	Randic molecular profiles
664	38	SP18	shape profile no. 18	Randic molecular profiles
665	39	SP19	shape profile no. 19	Randic molecular profiles

666	40	SP20	shape profile no. 20	Randic molecular profiles
667	41	SHP2	average shape profile index of order 2	Randic molecular profiles
668	1	W3D	3D-Wiener index	geometrical descriptors
669	2	J3D	3D-Balaban index	geometrical descriptors
670	3	H3D	3D-Harary index	geometrical descriptors
671	4	AGDD	average geometric distance degree	geometrical descriptors
672	5	DDI	D/D index	geometrical descriptors
673	6	ADDD	average distance/distance degree	geometrical descriptors
674	7	G1	gravitational index G1	geometrical descriptors
675	8	G2	gravitational index G2 (bond-restricted)	geometrical descriptors
676	9	RGyr	radius of gyration (mass weighted)	geometrical descriptors
677	10	SPAN	span R	geometrical descriptors
678	11	SPAM	average span R	geometrical descriptors
679	12	MEcc	molecular eccentricity	geometrical descriptors
680	13	SPH	sphericity	geometrical descriptors
681	14	ASP	asphericity	geometrical descriptors
682	15	FDI	folding degree index	geometrical descriptors
683	16	PJ13	3D Petitjean shape index	geometrical descriptors

684	17	L/Bw	length-to-breadth ratio by WHIM	geometrical descriptors
685	18	SEig	absolute eigenvalue sum on geometry matrix	geometrical descriptors
686	19	HOMA	Harmonic Oscillator Model of Aromaticity index	geometrical descriptors
687	20	RCI	Jug RC index	geometrical descriptors
688	21	AROM	aromaticity index	geometrical descriptors
689	22	HOMT	HOMA total	geometrical descriptors
690	23	DISPm	d COMMA2 value / weighted by atomic masses	geometrical descriptors
691	24	QXXm	Qxx COMMA2 value / weighted by atomic masses	geometrical descriptors
692	25	QYYm	Qyy COMMA2 value / weighted by atomic masses	geometrical descriptors
693	26	QZZm	Qzz COMMA2 value / weighted by atomic masses	geometrical descriptors
694	27	DISPv	d COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
695	28	QXXv	Qxx COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
696	29	QYYv	Qyy COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
697	30	QZZv	Qzz COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
698	31	DISPe	d COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
699	32	QXXe	Qxx COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
700	33	QYYe	Qyy COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
701	34	QZZe	Qzz COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors

702	35	DISPp	d COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
703	36	QXXp	Qxx COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
704	37	QYYp	Qyy COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
705	38	QZZp	Qzz COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
706	39	G(N..N)	sum of geometrical distances between N..N	geometrical descriptors
707	40	G(N..O)	sum of geometrical distances between N..O	geometrical descriptors
708	41	G(N..S)	sum of geometrical distances between N..S	geometrical descriptors
709	42	G(N..P)	sum of geometrical distances between N..P	geometrical descriptors
710	43	G(N..F)	sum of geometrical distances between N..F	geometrical descriptors
711	44	G(N..Cl)	sum of geometrical distances between N..Cl	geometrical descriptors
712	45	G(N..Br)	sum of geometrical distances between N..Br	geometrical descriptors
713	46	G(N..I)	sum of geometrical distances between N..I	geometrical descriptors
714	47	G(O..O)	sum of geometrical distances between O..O	geometrical descriptors
715	48	G(O..S)	sum of geometrical distances between O..S	geometrical descriptors
716	49	G(O..P)	sum of geometrical distances between O..P	geometrical descriptors
717	50	G(O..F)	sum of geometrical distances between O..F	geometrical descriptors
718	51	G(O..Cl)	sum of geometrical distances between O..Cl	geometrical descriptors
719	52	G(O..Br)	sum of geometrical distances between O..Br	geometrical descriptors

720	53	G(O..I)	sum of geometrical distances between O..I	geometrical descriptors
721	54	G(S..S)	sum of geometrical distances between S..S	geometrical descriptors
722	55	G(S..P)	sum of geometrical distances between S..P	geometrical descriptors
723	56	G(S..F)	sum of geometrical distances between S..F	geometrical descriptors
724	57	G(S..Cl)	sum of geometrical distances between S..Cl	geometrical descriptors
725	58	G(S..Br)	sum of geometrical distances between S..Br	geometrical descriptors
726	59	G(S..I)	sum of geometrical distances between S..I	geometrical descriptors
727	60	G(P..P)	sum of geometrical distances between P..P	geometrical descriptors
728	61	G(P..F)	sum of geometrical distances between P..F	geometrical descriptors
729	62	G(P..Cl)	sum of geometrical distances between P..Cl	geometrical descriptors
730	63	G(P..Br)	sum of geometrical distances between P..Br	geometrical descriptors
731	64	G(P..I)	sum of geometrical distances between P..I	geometrical descriptors
732	65	G(F..F)	sum of geometrical distances between F..F	geometrical descriptors
733	66	G(F..Cl)	sum of geometrical distances between F..Cl	geometrical descriptors
734	67	G(F..Br)	sum of geometrical distances between F..Br	geometrical descriptors
735	68	G(F..I)	sum of geometrical distances between F..I	geometrical descriptors
736	69	G(Cl..Cl)	sum of geometrical distances between Cl..Cl	geometrical descriptors
737	70	G(Cl..Br)	sum of geometrical distances between Cl..Br	geometrical descriptors

738	71	G(Cl..l)	sum of geometrical distances between Cl..l	geometrical descriptors
739	72	G(Br..Br)	sum of geometrical distances between Br..Br	geometrical descriptors
740	73	G(Br..l)	sum of geometrical distances between Br..l	geometrical descriptors
741	74	G(l..l)	sum of geometrical distances between l..l	geometrical descriptors
742	1	RDF010u	Radial Distribution Function - 1.0 / unweighted	RDF descriptors
743	2	RDF015u	Radial Distribution Function - 1.5 / unweighted	RDF descriptors
744	3	RDF020u	Radial Distribution Function - 2.0 / unweighted	RDF descriptors
745	4	RDF025u	Radial Distribution Function - 2.5 / unweighted	RDF descriptors
746	5	RDF030u	Radial Distribution Function - 3.0 / unweighted	RDF descriptors
747	6	RDF035u	Radial Distribution Function - 3.5 / unweighted	RDF descriptors
748	7	RDF040u	Radial Distribution Function - 4.0 / unweighted	RDF descriptors
749	8	RDF045u	Radial Distribution Function - 4.5 / unweighted	RDF descriptors
750	9	RDF050u	Radial Distribution Function - 5.0 / unweighted	RDF descriptors
751	10	RDF055u	Radial Distribution Function - 5.5 / unweighted	RDF descriptors
752	11	RDF060u	Radial Distribution Function - 6.0 / unweighted	RDF descriptors
753	12	RDF065u	Radial Distribution Function - 6.5 / unweighted	RDF descriptors
754	13	RDF070u	Radial Distribution Function - 7.0 / unweighted	RDF descriptors
755	14	RDF075u	Radial Distribution Function - 7.5 / unweighted	RDF descriptors

756	15	RDF080u	Radial Distribution Function - 8.0 / unweighted RDF descriptors
757	16	RDF085u	Radial Distribution Function - 8.5 / unweighted RDF descriptors
758	17	RDF090u	Radial Distribution Function - 9.0 / unweighted RDF descriptors
759	18	RDF095u	Radial Distribution Function - 9.5 / unweighted RDF descriptors
760	19	RDF100u	Radial Distribution Function - 10.0 / unweighted RDF descriptors
761	20	RDF105u	Radial Distribution Function - 10.5 / unweighted RDF descriptors
762	21	RDF110u	Radial Distribution Function - 11.0 / unweighted RDF descriptors
763	22	RDF115u	Radial Distribution Function - 11.5 / unweighted RDF descriptors
764	23	RDF120u	Radial Distribution Function - 12.0 / unweighted RDF descriptors
765	24	RDF125u	Radial Distribution Function - 12.5 / unweighted RDF descriptors
766	25	RDF130u	Radial Distribution Function - 13.0 / unweighted RDF descriptors
767	26	RDF135u	Radial Distribution Function - 13.5 / unweighted RDF descriptors
768	27	RDF140u	Radial Distribution Function - 14.0 / unweighted RDF descriptors
769	28	RDF145u	Radial Distribution Function - 14.5 / unweighted RDF descriptors
770	29	RDF150u	Radial Distribution Function - 15.0 / unweighted RDF descriptors
771	30	RDF155u	Radial Distribution Function - 15.5 / unweighted RDF descriptors
772	31	RDF010m	Radial Distribution Function - 1.0 / weighted by atomic masses RDF descriptors
773	32	RDF015m	Radial Distribution Function - 1.5 / weighted by atomic masses RDF descriptors

774	33	RDF020m	Radial Distribution Function - 2.0 / weighted by atomic masses	RDF descriptors
775	34	RDF025m	Radial Distribution Function - 2.5 / weighted by atomic masses	RDF descriptors
776	35	RDF030m	Radial Distribution Function - 3.0 / weighted by atomic masses	RDF descriptors
777	36	RDF035m	Radial Distribution Function - 3.5 / weighted by atomic masses	RDF descriptors
778	37	RDF040m	Radial Distribution Function - 4.0 / weighted by atomic masses	RDF descriptors
779	38	RDF045m	Radial Distribution Function - 4.5 / weighted by atomic masses	RDF descriptors
780	39	RDF050m	Radial Distribution Function - 5.0 / weighted by atomic masses	RDF descriptors
781	40	RDF055m	Radial Distribution Function - 5.5 / weighted by atomic masses	RDF descriptors
782	41	RDF060m	Radial Distribution Function - 6.0 / weighted by atomic masses	RDF descriptors
783	42	RDF065m	Radial Distribution Function - 6.5 / weighted by atomic masses	RDF descriptors
784	43	RDF070m	Radial Distribution Function - 7.0 / weighted by atomic masses	RDF descriptors
785	44	RDF075m	Radial Distribution Function - 7.5 / weighted by atomic masses	RDF descriptors
786	45	RDF080m	Radial Distribution Function - 8.0 / weighted by atomic masses	RDF descriptors
787	46	RDF085m	Radial Distribution Function - 8.5 / weighted by atomic masses	RDF descriptors
788	47	RDF090m	Radial Distribution Function - 9.0 / weighted by atomic masses	RDF descriptors
789	48	RDF095m	Radial Distribution Function - 9.5 / weighted by atomic masses	RDF descriptors
790	49	RDF100m	Radial Distribution Function - 10.0 / weighted by atomic masses	RDF descriptors
791	50	RDF105m	Radial Distribution Function - 10.5 / weighted by atomic masses	RDF descriptors

792	51	RDF110m	Radial Distribution Function - 11.0 / weighted by atomic masses	RDF descriptors
793	52	RDF115m	Radial Distribution Function - 11.5 / weighted by atomic masses	RDF descriptors
794	53	RDF120m	Radial Distribution Function - 12.0 / weighted by atomic masses	RDF descriptors
795	54	RDF125m	Radial Distribution Function - 12.5 / weighted by atomic masses	RDF descriptors
796	55	RDF130m	Radial Distribution Function - 13.0 / weighted by atomic masses	RDF descriptors
797	56	RDF135m	Radial Distribution Function - 13.5 / weighted by atomic masses	RDF descriptors
798	57	RDF140m	Radial Distribution Function - 14.0 / weighted by atomic masses	RDF descriptors
799	58	RDF145m	Radial Distribution Function - 14.5 / weighted by atomic masses	RDF descriptors
800	59	RDF150m	Radial Distribution Function - 15.0 / weighted by atomic masses	RDF descriptors
801	60	RDF155m	Radial Distribution Function - 15.5 / weighted by atomic masses	RDF descriptors
802	61	RDF010v	Radial Distribution Function - 1.0 / weighted by atomic van der Waals volumes	RDF descriptors
803	62	RDF015v	Radial Distribution Function - 1.5 / weighted by atomic van der Waals volumes	RDF descriptors
804	63	RDF020v	Radial Distribution Function - 2.0 / weighted by atomic van der Waals volumes	RDF descriptors
805	64	RDF025v	Radial Distribution Function - 2.5 / weighted by atomic van der Waals volumes	RDF descriptors
806	65	RDF030v	Radial Distribution Function - 3.0 / weighted by atomic van der Waals volumes	RDF descriptors
807	66	RDF035v	Radial Distribution Function - 3.5 / weighted by atomic van der Waals volumes	RDF descriptors
808	67	RDF040v	Radial Distribution Function - 4.0 / weighted by atomic van der Waals volumes	RDF descriptors
809	68	RDF045v	Radial Distribution Function - 4.5 / weighted by atomic van der Waals volumes	RDF descriptors

810	69	RDF050v	Radial Distribution Function - 5.0 / weighted by atomic van der Waals volumes	RDF descriptors
811	70	RDF055v	Radial Distribution Function - 5.5 / weighted by atomic van der Waals volumes	RDF descriptors
812	71	RDF060v	Radial Distribution Function - 6.0 / weighted by atomic van der Waals volumes	RDF descriptors
813	72	RDF065v	Radial Distribution Function - 6.5 / weighted by atomic van der Waals volumes	RDF descriptors
814	73	RDF070v	Radial Distribution Function - 7.0 / weighted by atomic van der Waals volumes	RDF descriptors
815	74	RDF075v	Radial Distribution Function - 7.5 / weighted by atomic van der Waals volumes	RDF descriptors
816	75	RDF080v	Radial Distribution Function - 8.0 / weighted by atomic van der Waals volumes	RDF descriptors
817	76	RDF085v	Radial Distribution Function - 8.5 / weighted by atomic van der Waals volumes	RDF descriptors
818	77	RDF090v	Radial Distribution Function - 9.0 / weighted by atomic van der Waals volumes	RDF descriptors
819	78	RDF095v	Radial Distribution Function - 9.5 / weighted by atomic van der Waals volumes	RDF descriptors
820	79	RDF100v	Radial Distribution Function - 10.0 / weighted by atomic van der Waals volumes	RDF descriptors
821	80	RDF105v	Radial Distribution Function - 10.5 / weighted by atomic van der Waals volumes	RDF descriptors
822	81	RDF110v	Radial Distribution Function - 11.0 / weighted by atomic van der Waals volumes	RDF descriptors
823	82	RDF115v	Radial Distribution Function - 11.5 / weighted by atomic van der Waals volumes	RDF descriptors
824	83	RDF120v	Radial Distribution Function - 12.0 / weighted by atomic van der Waals volumes	RDF descriptors
825	84	RDF125v	Radial Distribution Function - 12.5 / weighted by atomic van der Waals volumes	RDF descriptors
826	85	RDF130v	Radial Distribution Function - 13.0 / weighted by atomic van der Waals volumes	RDF descriptors
827	86	RDF135v	Radial Distribution Function - 13.5 / weighted by atomic van der Waals volumes	RDF descriptors

828	87	RDF140v	Radial Distribution Function - 14.0 / weighted by atomic van der Waals volumes	RDF descriptors
829	88	RDF145v	Radial Distribution Function - 14.5 / weighted by atomic van der Waals volumes	RDF descriptors
830	89	RDF150v	Radial Distribution Function - 15.0 / weighted by atomic van der Waals volumes	RDF descriptors
831	90	RDF155v	Radial Distribution Function - 15.5 / weighted by atomic van der Waals volumes	RDF descriptors
832	91	RDF010e	Radial Distribution Function - 1.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
833	92	RDF015e	Radial Distribution Function - 1.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
834	93	RDF020e	Radial Distribution Function - 2.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
835	94	RDF025e	Radial Distribution Function - 2.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
836	95	RDF030e	Radial Distribution Function - 3.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
837	96	RDF035e	Radial Distribution Function - 3.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
838	97	RDF040e	Radial Distribution Function - 4.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
839	98	RDF045e	Radial Distribution Function - 4.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
840	99	RDF050e	Radial Distribution Function - 5.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
841	100	RDF055e	Radial Distribution Function - 5.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
842	101	RDF060e	Radial Distribution Function - 6.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
843	102	RDF065e	Radial Distribution Function - 6.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
844	103	RDF070e	Radial Distribution Function - 7.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
845	104	RDF075e	Radial Distribution Function - 7.5 / weighted by atomic Sanderson electronegativities	RDF descriptors

846	105	RDF080e	Radial Distribution Function - 8.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
847	106	RDF085e	Radial Distribution Function - 8.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
848	107	RDF090e	Radial Distribution Function - 9.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
849	108	RDF095e	Radial Distribution Function - 9.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
850	109	RDF100e	Radial Distribution Function - 10.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
851	110	RDF105e	Radial Distribution Function - 10.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
852	111	RDF110e	Radial Distribution Function - 11.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
853	112	RDF115e	Radial Distribution Function - 11.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
854	113	RDF120e	Radial Distribution Function - 12.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
855	114	RDF125e	Radial Distribution Function - 12.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
856	115	RDF130e	Radial Distribution Function - 13.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
857	116	RDF135e	Radial Distribution Function - 13.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
858	117	RDF140e	Radial Distribution Function - 14.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
859	118	RDF145e	Radial Distribution Function - 14.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
860	119	RDF150e	Radial Distribution Function - 15.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
861	120	RDF155e	Radial Distribution Function - 15.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
862	121	RDF010p	Radial Distribution Function - 1.0 / weighted by atomic polarizabilities	RDF descriptors
863	122	RDF015p	Radial Distribution Function - 1.5 / weighted by atomic polarizabilities	RDF descriptors

864	123	RDF020p	Radial Distribution Function - 2.0 / weighted by atomic polarizabilities	RDF descriptors
865	124	RDF025p	Radial Distribution Function - 2.5 / weighted by atomic polarizabilities	RDF descriptors
866	125	RDF030p	Radial Distribution Function - 3.0 / weighted by atomic polarizabilities	RDF descriptors
867	126	RDF035p	Radial Distribution Function - 3.5 / weighted by atomic polarizabilities	RDF descriptors
868	127	RDF040p	Radial Distribution Function - 4.0 / weighted by atomic polarizabilities	RDF descriptors
869	128	RDF045p	Radial Distribution Function - 4.5 / weighted by atomic polarizabilities	RDF descriptors
870	129	RDF050p	Radial Distribution Function - 5.0 / weighted by atomic polarizabilities	RDF descriptors
871	130	RDF055p	Radial Distribution Function - 5.5 / weighted by atomic polarizabilities	RDF descriptors
872	131	RDF060p	Radial Distribution Function - 6.0 / weighted by atomic polarizabilities	RDF descriptors
873	132	RDF065p	Radial Distribution Function - 6.5 / weighted by atomic polarizabilities	RDF descriptors
874	133	RDF070p	Radial Distribution Function - 7.0 / weighted by atomic polarizabilities	RDF descriptors
875	134	RDF075p	Radial Distribution Function - 7.5 / weighted by atomic polarizabilities	RDF descriptors
876	135	RDF080p	Radial Distribution Function - 8.0 / weighted by atomic polarizabilities	RDF descriptors
877	136	RDF085p	Radial Distribution Function - 8.5 / weighted by atomic polarizabilities	RDF descriptors
878	137	RDF090p	Radial Distribution Function - 9.0 / weighted by atomic polarizabilities	RDF descriptors
879	138	RDF095p	Radial Distribution Function - 9.5 / weighted by atomic polarizabilities	RDF descriptors
880	139	RDF100p	Radial Distribution Function - 10.0 / weighted by atomic polarizabilities	RDF descriptors
881	140	RDF105p	Radial Distribution Function - 10.5 / weighted by atomic polarizabilities	RDF descriptors

882	141	RDF110p	Radial Distribution Function - 11.0 / weighted by atomic polarizabilities RDF descriptors
883	142	RDF115p	Radial Distribution Function - 11.5 / weighted by atomic polarizabilities RDF descriptors
884	143	RDF120p	Radial Distribution Function - 12.0 / weighted by atomic polarizabilities RDF descriptors
885	144	RDF125p	Radial Distribution Function - 12.5 / weighted by atomic polarizabilities RDF descriptors
886	145	RDF130p	Radial Distribution Function - 13.0 / weighted by atomic polarizabilities RDF descriptors
887	146	RDF135p	Radial Distribution Function - 13.5 / weighted by atomic polarizabilities RDF descriptors
888	147	RDF140p	Radial Distribution Function - 14.0 / weighted by atomic polarizabilities RDF descriptors
889	148	RDF145p	Radial Distribution Function - 14.5 / weighted by atomic polarizabilities RDF descriptors
890	149	RDF150p	Radial Distribution Function - 15.0 / weighted by atomic polarizabilities RDF descriptors
891	150	RDF155p	Radial Distribution Function - 15.5 / weighted by atomic polarizabilities RDF descriptors
892	1	Mor01u	3D-MoRSE - signal 01 / unweighted 3D-MoRSE descriptors
893	2	Mor02u	3D-MoRSE - signal 02 / unweighted 3D-MoRSE descriptors
894	3	Mor03u	3D-MoRSE - signal 03 / unweighted 3D-MoRSE descriptors
895	4	Mor04u	3D-MoRSE - signal 04 / unweighted 3D-MoRSE descriptors
896	5	Mor05u	3D-MoRSE - signal 05 / unweighted 3D-MoRSE descriptors
897	6	Mor06u	3D-MoRSE - signal 06 / unweighted 3D-MoRSE descriptors
898	7	Mor07u	3D-MoRSE - signal 07 / unweighted 3D-MoRSE descriptors
899	8	Mor08u	3D-MoRSE - signal 08 / unweighted 3D-MoRSE descriptors

900	9	Mor09u	3D-MoRSE - signal 09 / unweighted	3D-MoRSE descriptors
901	10	Mor10u	3D-MoRSE - signal 10 / unweighted	3D-MoRSE descriptors
902	11	Mor11u	3D-MoRSE - signal 11 / unweighted	3D-MoRSE descriptors
903	12	Mor12u	3D-MoRSE - signal 12 / unweighted	3D-MoRSE descriptors
904	13	Mor13u	3D-MoRSE - signal 13 / unweighted	3D-MoRSE descriptors
905	14	Mor14u	3D-MoRSE - signal 14 / unweighted	3D-MoRSE descriptors
906	15	Mor15u	3D-MoRSE - signal 15 / unweighted	3D-MoRSE descriptors
907	16	Mor16u	3D-MoRSE - signal 16 / unweighted	3D-MoRSE descriptors
908	17	Mor17u	3D-MoRSE - signal 17 / unweighted	3D-MoRSE descriptors
909	18	Mor18u	3D-MoRSE - signal 18 / unweighted	3D-MoRSE descriptors
910	19	Mor19u	3D-MoRSE - signal 19 / unweighted	3D-MoRSE descriptors
911	20	Mor20u	3D-MoRSE - signal 20 / unweighted	3D-MoRSE descriptors
912	21	Mor21u	3D-MoRSE - signal 21 / unweighted	3D-MoRSE descriptors
913	22	Mor22u	3D-MoRSE - signal 22 / unweighted	3D-MoRSE descriptors
914	23	Mor23u	3D-MoRSE - signal 23 / unweighted	3D-MoRSE descriptors
915	24	Mor24u	3D-MoRSE - signal 24 / unweighted	3D-MoRSE descriptors
916	25	Mor25u	3D-MoRSE - signal 25 / unweighted	3D-MoRSE descriptors
917	26	Mor26u	3D-MoRSE - signal 26 / unweighted	3D-MoRSE descriptors

918	27	Mor27u	3D-MoRSE - signal 27 / unweighted	3D-MoRSE descriptors
919	28	Mor28u	3D-MoRSE - signal 28 / unweighted	3D-MoRSE descriptors
920	29	Mor29u	3D-MoRSE - signal 29 / unweighted	3D-MoRSE descriptors
921	30	Mor30u	3D-MoRSE - signal 30 / unweighted	3D-MoRSE descriptors
922	31	Mor31u	3D-MoRSE - signal 31 / unweighted	3D-MoRSE descriptors
923	32	Mor32u	3D-MoRSE - signal 32 / unweighted	3D-MoRSE descriptors
924	33	Mor01m	3D-MoRSE - signal 01 / weighted by atomic masses	3D-MoRSE descriptors
925	34	Mor02m	3D-MoRSE - signal 02 / weighted by atomic masses	3D-MoRSE descriptors
926	35	Mor03m	3D-MoRSE - signal 03 / weighted by atomic masses	3D-MoRSE descriptors
927	36	Mor04m	3D-MoRSE - signal 04 / weighted by atomic masses	3D-MoRSE descriptors
928	37	Mor05m	3D-MoRSE - signal 05 / weighted by atomic masses	3D-MoRSE descriptors
929	38	Mor06m	3D-MoRSE - signal 06 / weighted by atomic masses	3D-MoRSE descriptors
930	39	Mor07m	3D-MoRSE - signal 07 / weighted by atomic masses	3D-MoRSE descriptors
931	40	Mor08m	3D-MoRSE - signal 08 / weighted by atomic masses	3D-MoRSE descriptors
932	41	Mor09m	3D-MoRSE - signal 09 / weighted by atomic masses	3D-MoRSE descriptors
933	42	Mor10m	3D-MoRSE - signal 10 / weighted by atomic masses	3D-MoRSE descriptors
934	43	Mor11m	3D-MoRSE - signal 11 / weighted by atomic masses	3D-MoRSE descriptors
935	44	Mor12m	3D-MoRSE - signal 12 / weighted by atomic masses	3D-MoRSE descriptors

936	45	Mor13m	3D-MoRSE - signal 13 / weighted by atomic masses	3D-MoRSE descriptors
937	46	Mor14m	3D-MoRSE - signal 14 / weighted by atomic masses	3D-MoRSE descriptors
938	47	Mor15m	3D-MoRSE - signal 15 / weighted by atomic masses	3D-MoRSE descriptors
939	48	Mor16m	3D-MoRSE - signal 16 / weighted by atomic masses	3D-MoRSE descriptors
940	49	Mor17m	3D-MoRSE - signal 17 / weighted by atomic masses	3D-MoRSE descriptors
941	50	Mor18m	3D-MoRSE - signal 18 / weighted by atomic masses	3D-MoRSE descriptors
942	51	Mor19m	3D-MoRSE - signal 19 / weighted by atomic masses	3D-MoRSE descriptors
943	52	Mor20m	3D-MoRSE - signal 20 / weighted by atomic masses	3D-MoRSE descriptors
944	53	Mor21m	3D-MoRSE - signal 21 / weighted by atomic masses	3D-MoRSE descriptors
945	54	Mor22m	3D-MoRSE - signal 22 / weighted by atomic masses	3D-MoRSE descriptors
946	55	Mor23m	3D-MoRSE - signal 23 / weighted by atomic masses	3D-MoRSE descriptors
947	56	Mor24m	3D-MoRSE - signal 24 / weighted by atomic masses	3D-MoRSE descriptors
948	57	Mor25m	3D-MoRSE - signal 25 / weighted by atomic masses	3D-MoRSE descriptors
949	58	Mor26m	3D-MoRSE - signal 26 / weighted by atomic masses	3D-MoRSE descriptors
950	59	Mor27m	3D-MoRSE - signal 27 / weighted by atomic masses	3D-MoRSE descriptors
951	60	Mor28m	3D-MoRSE - signal 28 / weighted by atomic masses	3D-MoRSE descriptors
952	61	Mor29m	3D-MoRSE - signal 29 / weighted by atomic masses	3D-MoRSE descriptors
953	62	Mor30m	3D-MoRSE - signal 30 / weighted by atomic masses	3D-MoRSE descriptors

954	63	Mor31m	3D-MoRSE - signal 31 / weighted by atomic masses	3D-MoRSE descriptors
955	64	Mor32m	3D-MoRSE - signal 32 / weighted by atomic masses	3D-MoRSE descriptors
956	65	Mor01v3D-MoRSE	- signal 01 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
957	66	Mor02v3D-MoRSE	- signal 02 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
958	67	Mor03v3D-MoRSE	- signal 03 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
959	68	Mor04v3D-MoRSE	- signal 04 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
960	69	Mor05v3D-MoRSE	- signal 05 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
961	70	Mor06v3D-MoRSE	- signal 06 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
962	71	Mor07v3D-MoRSE	- signal 07 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
963	72	Mor08v3D-MoRSE	- signal 08 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
964	73	Mor09v3D-MoRSE	- signal 09 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
965	74	Mor10v3D-MoRSE	- signal 10 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
966	75	Mor11v3D-MoRSE	- signal 11 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
967	76	Mor12v3D-MoRSE	- signal 12 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
968	77	Mor13v3D-MoRSE	- signal 13 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
969	78	Mor14v3D-MoRSE	- signal 14 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
970	79	Mor15v3D-MoRSE	- signal 15 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
971	80	Mor16v3D-MoRSE	- signal 16 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors

972	81	Mor17v3D-MoRSE - signal 17 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
973	82	Mor18v3D-MoRSE - signal 18 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
974	83	Mor19v3D-MoRSE - signal 19 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
975	84	Mor20v3D-MoRSE - signal 20 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
976	85	Mor21v3D-MoRSE - signal 21 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
977	86	Mor22v3D-MoRSE - signal 22 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
978	87	Mor23v3D-MoRSE - signal 23 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
979	88	Mor24v3D-MoRSE - signal 24 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
980	89	Mor25v3D-MoRSE - signal 25 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
981	90	Mor26v3D-MoRSE - signal 26 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
982	91	Mor27v3D-MoRSE - signal 27 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
983	92	Mor28v3D-MoRSE - signal 28 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
984	93	Mor29v3D-MoRSE - signal 29 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
985	94	Mor30v3D-MoRSE - signal 30 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
986	95	Mor31v3D-MoRSE - signal 31 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
987	96	Mor32v3D-MoRSE - signal 32 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
988	97	Mor01e 3D-MoRSE - signal 01 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
989	98	Mor02e 3D-MoRSE - signal 02 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors

990	99	Mor03e	3D-MoRSE - signal 03 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
991	100	Mor04e	3D-MoRSE - signal 04 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
992	101	Mor05e	3D-MoRSE - signal 05 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
993	102	Mor06e	3D-MoRSE - signal 06 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
994	103	Mor07e	3D-MoRSE - signal 07 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
995	104	Mor08e	3D-MoRSE - signal 08 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
996	105	Mor09e	3D-MoRSE - signal 09 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
997	106	Mor10e	3D-MoRSE - signal 10 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
998	107	Mor11e	3D-MoRSE - signal 11 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
999	108	Mor12e	3D-MoRSE - signal 12 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1000	109	Mor13e	3D-MoRSE - signal 13 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1001	110	Mor14e	3D-MoRSE - signal 14 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1002	111	Mor15e	3D-MoRSE - signal 15 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1003	112	Mor16e	3D-MoRSE - signal 16 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1004	113	Mor17e	3D-MoRSE - signal 17 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1005	114	Mor18e	3D-MoRSE - signal 18 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1006	115	Mor19e	3D-MoRSE - signal 19 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1007	116	Mor20e	3D-MoRSE - signal 20 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors

1008	117	Mor21e	3D-MoRSE - signal 21 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1009	118	Mor22e	3D-MoRSE - signal 22 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1010	119	Mor23e	3D-MoRSE - signal 23 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1011	120	Mor24e	3D-MoRSE - signal 24 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1012	121	Mor25e	3D-MoRSE - signal 25 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1013	122	Mor26e	3D-MoRSE - signal 26 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1014	123	Mor27e	3D-MoRSE - signal 27 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1015	124	Mor28e	3D-MoRSE - signal 28 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1016	125	Mor29e	3D-MoRSE - signal 29 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1017	126	Mor30e	3D-MoRSE - signal 30 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1018	127	Mor31e	3D-MoRSE - signal 31 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1019	128	Mor32e	3D-MoRSE - signal 32 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
1020	129	Mor01p	3D-MoRSE - signal 01 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1021	130	Mor02p	3D-MoRSE - signal 02 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1022	131	Mor03p	3D-MoRSE - signal 03 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1023	132	Mor04p	3D-MoRSE - signal 04 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1024	133	Mor05p	3D-MoRSE - signal 05 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1025	134	Mor06p	3D-MoRSE - signal 06 / weighted by atomic polarizabilities	3D-MoRSE descriptors

1026	135	Mor07p	3D-MoRSE - signal 07 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1027	136	Mor08p	3D-MoRSE - signal 08 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1028	137	Mor09p	3D-MoRSE - signal 09 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1029	138	Mor10p	3D-MoRSE - signal 10 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1030	139	Mor11p	3D-MoRSE - signal 11 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1031	140	Mor12p	3D-MoRSE - signal 12 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1032	141	Mor13p	3D-MoRSE - signal 13 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1033	142	Mor14p	3D-MoRSE - signal 14 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1034	143	Mor15p	3D-MoRSE - signal 15 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1035	144	Mor16p	3D-MoRSE - signal 16 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1036	145	Mor17p	3D-MoRSE - signal 17 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1037	146	Mor18p	3D-MoRSE - signal 18 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1038	147	Mor19p	3D-MoRSE - signal 19 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1039	148	Mor20p	3D-MoRSE - signal 20 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1040	149	Mor21p	3D-MoRSE - signal 21 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1041	150	Mor22p	3D-MoRSE - signal 22 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1042	151	Mor23p	3D-MoRSE - signal 23 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1043	152	Mor24p	3D-MoRSE - signal 24 / weighted by atomic polarizabilities	3D-MoRSE descriptors

1044	153	Mor25p	3D-MoRSE - signal 25 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1045	154	Mor26p	3D-MoRSE - signal 26 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1046	155	Mor27p	3D-MoRSE - signal 27 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1047	156	Mor28p	3D-MoRSE - signal 28 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1048	157	Mor29p	3D-MoRSE - signal 29 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1049	158	Mor30p	3D-MoRSE - signal 30 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1050	159	Mor31p	3D-MoRSE - signal 31 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1051	160	Mor32p	3D-MoRSE - signal 32 / weighted by atomic polarizabilities	3D-MoRSE descriptors
1052	1	L1u	1st component size directional WHIM index / unweighted	WHIM descriptors
1053	2	L2u	2nd component size directional WHIM index / unweighted	WHIM descriptors
1054	3	L3u	3rd component size directional WHIM index / unweighted	WHIM descriptors
1055	4	P1u	1st component shape directional WHIM index / unweighted	WHIM descriptors
1056	5	P2u	2nd component shape directional WHIM index / unweighted	WHIM descriptors
1057	6	G1u	1st component symmetry directional WHIM index / unweighted	WHIM descriptors
1058	7	G2u	2st component symmetry directional WHIM index / unweighted	WHIM descriptors
1059	8	G3u	3st component symmetry directional WHIM index / unweighted	WHIM descriptors
1060	9	E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
1061	10	E2u	2nd component accessibility directional WHIM index / unweighted	WHIM descriptors

1062	11	E3u	3rd component accessibility directional WHIM index / unweighted	WHIM descriptors
1063	12	L1m	1st component size directional WHIM index / weighted by atomic masses	WHIM descriptors
1064	13	L2m	2nd component size directional WHIM index / weighted by atomic masses	WHIM descriptors
1065	14	L3m	3rd component size directional WHIM index / weighted by atomic masses	WHIM descriptors
1066	15	P1m	1st component shape directional WHIM index / weighted by atomic masses	WHIM descriptors
1067	16	P2m	2nd component shape directional WHIM index / weighted by atomic masses	WHIM descriptors
1068	17	G1m	1st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors
1069	18	G2m	2st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors
1070	19	G3m	3st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors
1071	20	E1m	1st component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
1072	21	E2m	2nd component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
1073	22	E3m	3rd component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
1074	23	L1v	1st component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1075	24	L2v	2nd component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1076	25	L3v	3rd component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1077	26	P1v	1st component shape directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1078	27	P2v	2nd component shape directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1079	28	G1v	1st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors

1080	29	G2v	2st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1081	30	G3v	3st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1082	31	E1v	1st component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1083	32	E2v	2nd component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1084	33	E3v	3rd component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
1085	34	L1e	1st component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1086	35	L2e	2nd component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1087	36	L3e	3rd component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1088	37	P1e	1st component shape directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1089	38	P2e	2nd component shape directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1090	39	G1e	1st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1091	40	G2e	2st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1092	41	G3e	3st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1093	42	E1e	1st component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1094	43	E2e	2nd component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1095	44	E3e	3rd component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1096	45	L1p	1st component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1097	46	L2p	2nd component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors

1098	47	L3p	3rd component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1099	48	P1p	1st component shape directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1100	49	P2p	2nd component shape directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1101	50	G1p	1st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1102	51	G2p	2st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1103	52	G3p	3st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1104	53	E1p	1st component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1105	54	E2p	2nd component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1106	55	E3p	3rd component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1107	56	L1s	1st component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1108	57	L2s	2nd component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1109	58	L3s	3rd component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1110	59	P1s	1st component shape directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1111	60	P2s	2nd component shape directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1112	61	G1s	1st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1113	62	G2s	2st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1114	63	G3s	3st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1115	64	E1s	1st component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors

1116	65	E2s	2nd component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1117	66	E3s	3rd component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1118	67	Tu	T total size index / unweighted	WHIM descriptors
1119	68	Tm	T total size index / weighted by atomic masses	WHIM descriptors
1120	69	Tv	T total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1121	70	Te	T total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1122	71	Tp	T total size index / weighted by atomic polarizabilities	WHIM descriptors
1123	72	Ts	T total size index / weighted by atomic electrotopological states	WHIM descriptors
1124	73	Au	A total size index / unweighted	WHIM descriptors
1125	74	Am	A total size index / weighted by atomic masses	WHIM descriptors
1126	75	Av	A total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1127	76	Ae	A total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1128	77	Ap	A total size index / weighted by atomic polarizabilities	WHIM descriptors
1129	78	As	A total size index / weighted by atomic electrotopological states	WHIM descriptors
1130	79	Gu	G total symmetry index / unweighted	WHIM descriptors
1131	80	Gm	G total symmetry index / weighted by atomic masses	WHIM descriptors
1132	81	Gs	G total symmetry index / weighted by atomic electrotopological states	WHIM descriptors
1133	82	Ku	K global shape index / unweighted	WHIM descriptors

1134	83	Km	K global shape index / weighted by atomic masses	WHIM descriptors
1135	84	Kv	K global shape index / weighted by atomic van der Waals volumes	WHIM descriptors
1136	85	Ke	K global shape index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1137	86	Kp	K global shape index / weighted by atomic polarizabilities	WHIM descriptors
1138	87	Ks	K global shape index / weighted by atomic electrotopological states	WHIM descriptors
1139	88	Du	D total accessibility index / unweighted WHIM descriptors	
1140	89	Dm	D total accessibility index / weighted by atomic masses	WHIM descriptors
1141	90	Dv	D total accessibility index / weighted by atomic van der Waals volumes	WHIM descriptors
1142	91	De	D total accessibility index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1143	92	Dp	D total accessibility index / weighted by atomic polarizabilities	WHIM descriptors
1144	93	Ds	D total accessibility index / weighted by atomic electrotopological states	WHIM descriptors
1145	94	Vu	V total size index / unweighted WHIM descriptors	
1146	95	Vm	V total size index / weighted by atomic masses	WHIM descriptors
1147	96	Vv	V total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1148	97	Ve	V total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1149	98	Vp	V total size index / weighted by atomic polarizabilities	WHIM descriptors
1150	99	Vs	V total size index / weighted by atomic electrotopological states	WHIM descriptors
1151	1	ITH	total information content on the leverage equality	GETAWAY descriptors

1152	2	ISH	standardized information content on the leverage equality	GETAWAY descriptors
1153	3	HIC	mean information content on the leverage magnitude	GETAWAY descriptors
1154	4	HGM	geometric mean on the leverage magnitude	GETAWAY descriptors
1155	5	H0u	H autocorrelation of lag 0 / unweighted	GETAWAY descriptors
1156	6	H1u	H autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1157	7	H2u	H autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1158	8	H3u	H autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1159	9	H4u	H autocorrelation of lag 4 / unweighted	GETAWAY descriptors
1160	10	H5u	H autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1161	11	H6u	H autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1162	12	H7u	H autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1163	13	H8u	H autocorrelation of lag 8 / unweighted	GETAWAY descriptors
1164	14	HTu	H total index / unweighted	GETAWAY descriptors
1165	15	HATS0u	leverage-weighted autocorrelation of lag 0 / unweighted	GETAWAY descriptors
1166	16	HATS1u	leverage-weighted autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1167	17	HATS2u	leverage-weighted autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1168	18	HATS3u	leverage-weighted autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1169	19	HATS4u	leverage-weighted autocorrelation of lag 4 / unweighted	GETAWAY descriptors

1170	20	HATS5uleverage-weighted autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1171	21	HATS6uleverage-weighted autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1172	22	HATS7uleverage-weighted autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1173	23	HATS8uleverage-weighted autocorrelation of lag 8 / unweighted	GETAWAY descriptors
1174	24	HATSu leverage-weighted total index / unweighted	GETAWAY descriptors
1175	25	H0m H autocorrelation of lag 0 / weighted by atomic masses	GETAWAY descriptors
1176	26	H1m H autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1177	27	H2m H autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors
1178	28	H3m H autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1179	29	H4m H autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1180	30	H5m H autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1181	31	H6m H autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1182	32	H7m H autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1183	33	H8m H autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1184	34	HTm H total index / weighted by atomic masses	GETAWAY descriptors
1185	35	HATS0m leverage-weighted autocorrelation of lag 0 / weighted by atomic masses	GETAWAY descriptors
1186	36	HATS1m leverage-weighted autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1187	37	HATS2m leverage-weighted autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors

1188	38	HATS3m	leverage-weighted autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1189	39	HATS4m	leverage-weighted autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1190	40	HATS5m	leverage-weighted autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1191	41	HATS6m	leverage-weighted autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1192	42	HATS7m	leverage-weighted autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1193	43	HATS8m	leverage-weighted autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1194	44	HATSm	leverage-weighted total index / weighted by atomic masses	GETAWAY descriptors
1195	45	H0v	H autocorrelation of lag 0 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1196	46	H1v	H autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1197	47	H2v	H autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1198	48	H3v	H autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1199	49	H4v	H autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1200	50	H5v	H autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1201	51	H6v	H autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1202	52	H7v	H autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1203	53	H8v	H autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1204	54	HTv	H total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1205	55	HATS0v	leverage-weighted autocorrelation of lag 0 / weighted by atomic van der Waals volumes	GETAWAY descriptors

1206	56	HATS1v	leverage-weighted autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1207	57	HATS2v	leverage-weighted autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1208	58	HATS3v	leverage-weighted autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1209	59	HATS4v	leverage-weighted autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1210	60	HATS5v	leverage-weighted autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1211	61	HATS6v	leverage-weighted autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1212	62	HATS7v	leverage-weighted autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1213	63	HATS8v	leverage-weighted autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1214	64	HATSv	leverage-weighted total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1215	65	H0e	H autocorrelation of lag 0 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1216	66	H1e	H autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1217	67	H2e	H autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1218	68	H3e	H autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1219	69	H4e	H autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1220	70	H5e	H autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1221	71	H6e	H autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1222	72	H7e	H autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1223	73	H8e	H autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors

1224	74	HTe	H total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1225	75	HATS0e	leverage-weighted autocorrelation of lag 0 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1226	76	HATS1e	leverage-weighted autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1227	77	HATS2e	leverage-weighted autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1228	78	HATS3e	leverage-weighted autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1229	79	HATS4e	leverage-weighted autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1230	80	HATS5e	leverage-weighted autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1231	81	HATS6e	leverage-weighted autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1232	82	HATS7e	leverage-weighted autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1233	83	HATS8e	leverage-weighted autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1234	84	HATSe	leverage-weighted total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1235	85	H0p	H autocorrelation of lag 0 / weighted by atomic polarizabilities	GETAWAY descriptors
1236	86	H1p	H autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1237	87	H2p	H autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1238	88	H3p	H autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1239	89	H4p	H autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1240	90	H5p	H autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1241	91	H6p	H autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors

1242	92	H7p	H autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1243	93	H8p	H autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1244	94	HTp	H total index / weighted by atomic polarizabilities	GETAWAY descriptors
1245	95	HATS0p	leverage-weighted autocorrelation of lag 0 / weighted by atomic polarizabilities	GETAWAY descriptors
1246	96	HATS1p	leverage-weighted autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1247	97	HATS2p	leverage-weighted autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1248	98	HATS3p	leverage-weighted autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1249	99	HATS4p	leverage-weighted autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1250	100	HATS5p	leverage-weighted autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1251	101	HATS6p	leverage-weighted autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1252	102	HATS7p	leverage-weighted autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1253	103	HATS8p	leverage-weighted autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1254	104	HATSp	leverage-weighted total index / weighted by atomic polarizabilities	GETAWAY descriptors
1255	105	RCON	Randic-type R matrix connectivity	GETAWAY descriptors
1256	106	RARS	R matrix average row sum	GETAWAY descriptors
1257	107	REIG	first eigenvalue of the R matrix	GETAWAY descriptors
1258	108	R1u	R autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1259	109	R2u	R autocorrelation of lag 2 / unweighted	GETAWAY descriptors

1260	110	R3u	R autocorrelation of lag 3 / unweighted GETAWAY descriptors
1261	111	R4u	R autocorrelation of lag 4 / unweighted GETAWAY descriptors
1262	112	R5u	R autocorrelation of lag 5 / unweighted GETAWAY descriptors
1263	113	R6u	R autocorrelation of lag 6 / unweighted GETAWAY descriptors
1264	114	R7u	R autocorrelation of lag 7 / unweighted GETAWAY descriptors
1265	115	R8u	R autocorrelation of lag 8 / unweighted GETAWAY descriptors
1266	116	RTu	R total index / unweighted GETAWAY descriptors
1267	117	R1u+	R maximal autocorrelation of lag 1 / unweighted GETAWAY descriptors
1268	118	R2u+	R maximal autocorrelation of lag 2 / unweighted GETAWAY descriptors
1269	119	R3u+	R maximal autocorrelation of lag 3 / unweighted GETAWAY descriptors
1270	120	R4u+	R maximal autocorrelation of lag 4 / unweighted GETAWAY descriptors
1271	121	R5u+	R maximal autocorrelation of lag 5 / unweighted GETAWAY descriptors
1272	122	R6u+	R maximal autocorrelation of lag 6 / unweighted GETAWAY descriptors
1273	123	R7u+	R maximal autocorrelation of lag 7 / unweighted GETAWAY descriptors
1274	124	R8u+	R maximal autocorrelation of lag 8 / unweighted GETAWAY descriptors
1275	125	RTu+	R maximal index / unweighted GETAWAY descriptors
1276	126	R1m	R autocorrelation of lag 1 / weighted by atomic masses GETAWAY descriptors
1277	127	R2m	R autocorrelation of lag 2 / weighted by atomic masses GETAWAY descriptors

1278	128	R3m	R autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1279	129	R4m	R autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1280	130	R5m	R autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1281	131	R6m	R autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1282	132	R7m	R autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1283	133	R8m	R autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1284	134	RTm	R total index / weighted by atomic masses	GETAWAY descriptors
1285	135	R1m+	R maximal autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1286	136	R2m+	R maximal autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors
1287	137	R3m+	R maximal autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1288	138	R4m+	R maximal autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1289	139	R5m+	R maximal autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1290	140	R6m+	R maximal autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1291	141	R7m+	R maximal autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1292	142	R8m+	R maximal autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1293	143	RTm+	R maximal index / weighted by atomic masses	GETAWAY descriptors
1294	144	R1v	R autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1295	145	R2v	R autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors

1296	146	R3v	R autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1297	147	R4v	R autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1298	148	R5v	R autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1299	149	R6v	R autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1300	150	R7v	R autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1301	151	R8v	R autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1302	152	RTv	R total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1303	153	R1v+	R maximal autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1304	154	R2v+	R maximal autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1305	155	R3v+	R maximal autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1306	156	R4v+	R maximal autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1307	157	R5v+	R maximal autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1308	158	R6v+	R maximal autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1309	159	R7v+	R maximal autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1310	160	R8v+	R maximal autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1311	161	RTv+	R maximal index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1312	162	R1e	R autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1313	163	R2e	R autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors

1314	164	R3e	R autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1315	165	R4e	R autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1316	166	R5e	R autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1317	167	R6e	R autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1318	168	R7e	R autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1319	169	R8e	R autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1320	170	RTe	R total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1321	171	R1e+	R maximal autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1322	172	R2e+	R maximal autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1323	173	R3e+	R maximal autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1324	174	R4e+	R maximal autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1325	175	R5e+	R maximal autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1326	176	R6e+	R maximal autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1327	177	R7e+	R maximal autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1328	178	R8e+	R maximal autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1329	179	RTe+	R maximal index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1330	180	R1p	R autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1331	181	R2p	R autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors

1332	182	R3p	R autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1333	183	R4p	R autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1334	184	R5p	R autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1335	185	R6p	R autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1336	186	R7p	R autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1337	187	R8p	R autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1338	188	RTp	R total index / weighted by atomic polarizabilities	GETAWAY descriptors
1339	189	R1p+	R maximal autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1340	190	R2p+	R maximal autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1341	191	R3p+	R maximal autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1342	192	R4p+	R maximal autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1343	193	R5p+	R maximal autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1344	194	R6p+	R maximal autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1345	195	R7p+	R maximal autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1346	196	R8p+	R maximal autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1347	197	RTp+	R maximal index / weighted by atomic polarizabilities	GETAWAY descriptors
1348	1	nCp	number of terminal primary C(sp ³)	functional group counts
1349	2	nCs	number of total secondary C(sp ³)	functional group counts

1350	3	nCt	number of total tertiary C(sp ³)	functional group counts
1351	4	nCq	number of total quaternary C(sp ³)	functional group counts
1352	5	nCrs	number of ring secondary C(sp ³)	functional group counts
1353	6	nCrt	number of ring tertiary C(sp ³)	functional group counts
1354	7	nCrq	number of ring quaternary C(sp ³)	functional group counts
1355	8	nCar	number of aromatic C(sp ²)	functional group counts
1356	9	nCbH	number of unsubstituted benzene C(sp ²)	functional group counts
1357	10	nCb-	number of substituted benzene C(sp ²)	functional group counts
1358	11	nCconj	number of non-aromatic conjugated C(sp ²)	functional group counts
1359	12	nR=Cp	number of terminal primary C(sp ²)	functional group counts
1360	13	nR=Cs	number of aliphatic secondary C(sp ²)	functional group counts
1361	14	nR=Ct	number of aliphatic tertiary C(sp ²)	functional group counts
1362	15	n=C=	number of allenes groups	functional group counts
1363	16	nR#CH/X	number of terminal C(sp)	functional group counts
1364	17	nR#C-	number of non-terminal C(sp)	functional group counts
1365	18	nROCN	number of cyanates (aliphatic)	functional group counts
1366	19	nArOCN	number of cyanates (aromatic)	functional group counts
1367	20	nRNCO	number of isocyanates (aliphatic)	functional group counts

1368	21	nArNCO	number of isocyanates (aromatic)	functional group counts
1369	22	nRSCN	number of thiocyanates (aliphatic)	functional group counts
1370	23	nArSCN	number of thiocyanates (aromatic)	functional group counts
1371	24	nRNCS	number of isothiocyanates (aliphatic)	functional group counts
1372	25	nArNCS	number of isothiocyanates (aromatic)	functional group counts
1373	26	nRCOOH	number of carboxylic acids (aliphatic)	functional group counts
1374	27	nArCOOH	number of carboxylic acids (aromatic)	functional group counts
1375	28	nRCOOR	number of esters (aliphatic)	functional group counts
1376	29	nArCOOR	number of esters (aromatic)	functional group counts
1377	30	nRCONH2	number of primary amides (aliphatic)	functional group counts
1378	31	nArCONH2	number of primary amides (aromatic)	functional group counts
1379	32	nRCONHR	number of secondary amides (aliphatic)	functional group counts
1380	33	nArCONHR	number of secondary amides (aromatic)	functional group counts
1381	34	nRCONR2	number of tertiary amides (aliphatic)	functional group counts
1382	35	nArCONR2	number of tertiary amides (aromatic)	functional group counts
1383	36	nROCON	number of (thio-) carbamates (aliphatic)	functional group counts
1384	37	nArOCON	number of (thio-) carbamates (aromatic)	functional group counts
1385	38	nRCOX	number of acyl halogenides (aliphatic)	functional group counts

1386	39	nArCOX	number of acyl halogenides (aromatic)	functional group counts
1387	40	nRCSOH	number of thioacids (aliphatic)	functional group counts
1388	41	nArCSOH	number of thioacids (aromatic)	functional group counts
1389	42	nRCSSH	number of dithioacids (aliphatic)	functional group counts
1390	43	nArCSSH	number of dithioacids (aromatic)	functional group counts
1391	44	nRCOSR	number of thioesters (aliphatic)	functional group counts
1392	45	nArCOSR	number of thioesters (aromatic)	functional group counts
1393	46	nRCSSR	number of dithioesters (aliphatic)	functional group counts
1394	47	nArCSSR	number of dithioesters (aromatic)	functional group counts
1395	48	nRCHO	number of aldehydes (aliphatic)	functional group counts
1396	49	nArCHO	number of aldehydes (aromatic)	functional group counts
1397	50	nRCO	number of ketones (aliphatic)	functional group counts
1398	51	nArCO	number of ketones (aromatic)	functional group counts
1399	52	nCONN	number of urea (-thio) derivatives	functional group counts
1400	53	nC=O(O)2	number of carbonate (-thio) derivatives	functional group counts
1401	54	nN=C-N<	number of amidine derivatives	functional group counts
1402	55	nC(=N)N2	number of guanidine derivatives	functional group counts
1403	56	nRC=N	number of imines (aliphatic)	functional group counts

1404	57	nArC=N	number of imines (aromatic)	functional group counts
1405	58	nRCNO	number of oximes (aliphatic)	functional group counts
1406	59	nArCNO	number of oximes (aromatic)	functional group counts
1407	60	nRNH2	number of primary amines (aliphatic)	functional group counts
1408	61	nArNH2	number of primary amines (aromatic)	functional group counts
1409	62	nRNHR	number of secondary amines (aliphatic)	functional group counts
1410	63	nArNHR	number of secondary amines (aromatic)	functional group counts
1411	64	nRNR2	number of tertiary amines (aliphatic)	functional group counts
1412	65	nArNR2	number of tertiary amines (aromatic)	functional group counts
1413	66	nN-N	number of N hydrazines	functional group counts
1414	67	nN=N	number of N azo-derivatives	functional group counts
1415	68	nRCN	number of nitriles (aliphatic)	functional group counts
1416	69	nArCN	number of nitriles (aromatic)	functional group counts
1417	70	nN+	number of positively charged N	functional group counts
1418	71	nNq	number of quaternary N	functional group counts
1419	72	nRNHO	number of hydroxylamines (aliphatic)	functional group counts
1420	73	nArNHO	number of hydroxylamines (aromatic)	functional group counts
1421	74	nRNNOx	number of N-nitroso groups (aliphatic)	functional group counts

1422	75	nArNNOx	number of N-nitroso groups (aromatic)	functional group counts
1423	76	nRNO	number of nitroso groups (aliphatic)	functional group counts
1424	77	nArNO	number of nitroso groups (aromatic)	functional group counts
1425	78	nRNO2	number of nitro groups (aliphatic)	functional group counts
1426	79	nArNO2	number of nitro groups (aromatic)	functional group counts
1427	80	nN(CO)2	number of imides (-thio)	functional group counts
1428	81	nC=N-N<	number of hydrazones	functional group counts
1429	82	nROH	number of hydroxyl groups	functional group counts
1430	83	nArOH	number of aromatic hydroxyls	functional group counts
1431	84	nOHp	number of primary alcohols	functional group counts
1432	85	nOHs	number of secondary alcohols	functional group counts
1433	86	nOHt	number of tertiary alcohols	functional group counts
1434	87	nROR	number of ethers (aliphatic)	functional group counts
1435	88	nArOR	number of ethers (aromatic)	functional group counts
1436	89	nROX	number of hypohalogenides (aliphatic)	functional group counts
1437	90	nArOX	number of hypohalogenides (aromatic)	functional group counts
1438	91	nO(C=O)2	number of anhydrides (-thio)	functional group counts
1439	92	nH2O	number of water molecules	functional group counts

1440	93	nSH	number of thiols	functional group counts
1441	94	nC=S	number of thioketones	functional group counts
1442	95	nRSR	number of sulfides	functional group counts
1443	96	nRSSR	number of disulfides	functional group counts
1444	97	nSO	number of sulfoxides	functional group counts
1445	98	nS(=O)2	number of sulfones	functional group counts
1446	99	nSOH	number of sulfenic (thio-) acids	functional group counts
1447	100	nSOOH	number of sulfinic (thio-/dithio-) acids	functional group counts
1448	101	nSO2OH	number of sulfonic (thio-/dithio-) acids	functional group counts
1449	102	nSO3OH	number of sulfuric (thio-/dithio-) acids	functional group counts
1450	103	nSO2	number of sulfites (thio-/dithio-)	functional group counts
1451	104	nSO3	number of sulfonates (thio-/dithio-)	functional group counts
1452	105	nSO4	number of sulfates (thio-/dithio-)	functional group counts
1453	106	nSO2N	number of sulfonamides (thio-/dithio-)	functional group counts
1454	107	nPO3	number of phosphites/thiophosphites	functional group counts
1455	108	nPO4	number of phosphates/thiophosphates	functional group counts
1456	109	nPR3	number of phosphanes	functional group counts
1457	110	nP(=O)O2R	number of phosphonates (thio-)	functional group counts

1458	111	nP(=O)R3/nPR5	number of phosphoranes (thio-)	functional group counts
1459	112	nCH2RX	number of CH2RX	functional group counts
1460	113	nCHR2X	number of CHR2X	functional group counts
1461	114	nCR3X	number of CR3X	functional group counts
1462	115	nR=CHX	number of R=CHX	functional group counts
1463	116	nR=CRX	number of R=CRX	functional group counts
1464	117	nR#CX	number of R#CX	functional group counts
1465	118	nCHRX2	number of CHRX2	functional group counts
1466	119	nCR2X2	number of CR2X2	functional group counts
1467	120	nR=CX2	number of R=CX2	functional group counts
1468	121	nCRX3	number of CRX3	functional group counts
1469	122	nArX	number of X on aromatic ring	functional group counts
1470	123	nCXr	number of X on ring C(sp3)	functional group counts
1471	124	nCXr=	number of X on ring C(sp2)	functional group counts
1472	125	nCconjX	number of X on exo-conjugated C	functional group counts
1473	126	nAziridines	number of Aziridines	functional group counts
1474	127	nOxiranes	number of Oxiranes	functional group counts
1475	128	nThiranes	number of Thiranes	functional group counts

1476	129	nAzetidines	number of Azetidines	functional group counts
1477	130	nOxetanes	number of Oxetanes	functional group counts
1478	131	nThioethanes	number of Thioethanes	functional group counts
1479	132	nBeta-Lactams	number of Beta-Lactams	functional group counts
1480	133	nPyrrolidines	number of Pyrrolidines	functional group counts
1481	134	nOxolanes	number of Oxolanes	functional group counts
1482	135	ntH-Thiophenes	number of tetrahydro-thiophenes	functional group counts
1483	136	nPyrroles	number of Pyrroles	functional group counts
1484	137	nPyrazoles	number of Pyrazoles	functional group counts
1485	138	nImidazoles	number of Imidazoles	functional group counts
1486	139	nFuranes	number of Furanes	functional group counts
1487	140	nThiophenes	number of Thiophenes	functional group counts
1488	141	nOxazoles	number of Oxazoles	functional group counts
1489	142	nIsoxazoles	number of Isoxazoles	functional group counts
1490	143	nThiazoles	number of Thiazoles	functional group counts
1491	144	nIsothiazoles	number of Isothiazoles	functional group counts
1492	145	nTriazoles	number of Triazoles	functional group counts
1493	146	nPyridines	number of Pyridines	functional group counts

1494	147	nPyridazines	number of Pyridazines	functional group counts
1495	148	nPyrimidines	number of Pyrimidines	functional group counts
1496	149	nPyrazines	number of Pyrazines	functional group counts
1497	150	n135-Triazines	number of 1-3-5-Triazines	functional group counts
1498	151	n124-Triazines	number of 1-2-4-Triazines	functional group counts
1499	152	nHDon	number of donor atoms for H-bonds (N and O)	functional group counts
1500	153	nHAcc	number of acceptor atoms for H-bonds (N,O,F)	functional group counts
1501	154	nHBonds	number of intramolecular H-bonds (with N,O,F)	functional group counts
1502	1	C-001	CH3R / CH4	atom-centred fragments
1503	2	C-002	CH2R2	atom-centred fragments
1504	3	C-003	CHR3	atom-centred fragments
1505	4	C-004	CR4	atom-centred fragments
1506	5	C-005	CH3X	atom-centred fragments
1507	6	C-006	CH2RX	atom-centred fragments
1508	7	C-007	CH2X2	atom-centred fragments
1509	8	C-008	CHR2X	atom-centred fragments
1510	9	C-009	CHRX2	atom-centred fragments
1511	10	C-010	CHX3	atom-centred fragments

1512	11	C-011	CR3X	atom-centred fragments
1513	12	C-012	CR2X2	atom-centred fragments
1514	13	C-013	CRX3	atom-centred fragments
1515	14	C-014	CX4	atom-centred fragments
1516	15	C-015	=CH2	atom-centred fragments
1517	16	C-016	=CHR	atom-centred fragments
1518	17	C-017	=CR2	atom-centred fragments
1519	18	C-018	=CHX	atom-centred fragments
1520	19	C-019	=CRX	atom-centred fragments
1521	20	C-020	=CX2	atom-centred fragments
1522	21	C-021	#CH	atom-centred fragments
1523	22	C-022	#CR / R=C=R	atom-centred fragments
1524	23	C-023	#CX	atom-centred fragments
1525	24	C-024	R--CH--R	atom-centred fragments
1526	25	C-025	R--CR--R	atom-centred fragments
1527	26	C-026	R--CX--R	atom-centred fragments
1528	27	C-027	R--CH--X	atom-centred fragments
1529	28	C-028	R--CR--X	atom-centred fragments

1530	29	C-029	R--CX--X	atom-centred fragments
1531	30	C-030	X--CH--X	atom-centred fragments
1532	31	C-031	X--CR--X	atom-centred fragments
1533	32	C-032	X--CX--X	atom-centred fragments
1534	33	C-033	R--CH..X	atom-centred fragments
1535	34	C-034	R--CR..X	atom-centred fragments
1536	35	C-035	R--CX..X	atom-centred fragments
1537	36	C-036	Al-CH=X	atom-centred fragments
1538	37	C-037	Ar-CH=X	atom-centred fragments
1539	38	C-038	Al-C(=X)-Al	atom-centred fragments
1540	39	C-039	Ar-C(=X)-R	atom-centred fragments
1541	40	C-040	R-C(=X)-X / R-C#X / X=C=X	atom-centred fragments
1542	41	C-041	X-C(=X)-X	atom-centred fragments
1543	42	C-042	X--CH..X	atom-centred fragments
1544	43	C-043	X--CR..X	atom-centred fragments
1545	44	C-044	X--CX..X	atom-centred fragments
1546	45	U-045	undefined	atom-centred fragments
1547	46	H-046	H attached to C0(sp3) no X attached to next C	atom-centred fragments

1548	47	H-047	H attached to C1(sp3)/C0(sp2)	atom-centred fragments
1549	48	H-048	H attached to C2(sp3)/C1(sp2)/C0(sp)	atom-centred fragments
1550	49	H-049	H attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)	atom-centred fragments
1551	50	H-050	H attached to heteroatom	atom-centred fragments
1552	51	H-051	H attached to alpha-C	atom-centred fragments
1553	52	H-052	H attached to C0(sp3) with 1X attached to next C	atom-centred fragments
1554	53	H-053	H attached to C0(sp3) with 2X attached to next C	atom-centred fragments
1555	54	H-054	H attached to C0(sp3) with 3X attached to next C	atom-centred fragments
1556	55	H-055	H attached to C0(sp3) with 4X attached to next C	atom-centred fragments
1557	56	O-056	alcohol	atom-centred fragments
1558	57	O-057	phenol / enol / carboxyl OH	atom-centred fragments
1559	58	O-058	=O	atom-centred fragments
1560	59	O-059	Al-O-Al	atom-centred fragments
1561	60	O-060	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X	atom-centred fragments
1562	61	O-061	O--	atom-centred fragments
1563	62	O-062	O- (negatively charged)	atom-centred fragments
1564	63	O-063	R-O-O-R	atom-centred fragments
1565	64	Se-064	Any-Se-Any	atom-centred fragments

1566	65	Se-065	=Se	atom-centred fragments
1567	66	N-066	Al-NH ₂	atom-centred fragments
1568	67	N-067	Al ₂ -NH	atom-centred fragments
1569	68	N-068	Al ₃ -N	atom-centred fragments
1570	69	N-069	Ar-NH ₂ / X-NH ₂	atom-centred fragments
1571	70	N-070	Ar-NH-Al	atom-centred fragments
1572	71	N-071	Ar-NAl ₂	atom-centred fragments
1573	72	N-072	RCO-N< / >N-X=X	atom-centred fragments
1574	73	N-073	Ar ₂ NH / Ar ₃ N / Ar ₂ N-Al / R..N..R	atom-centred fragments
1575	74	N-074	R#N / R=N-	atom-centred fragments
1576	75	N-075	R--N--R / R--N--X	atom-centred fragments
1577	76	N-076	Ar-NO ₂ / R--N(--R)--O / RO-NO	atom-centred fragments
1578	77	N-077	Al-NO ₂	atom-centred fragments
1579	78	N-078	Ar-N=X / X-N=X	atom-centred fragments
1580	79	N-079	N ⁺ (positively charged)	atom-centred fragments
1581	80	U-080	undefined	atom-centred fragments
1582	81	F-081	F attached to C1(sp ³)	atom-centred fragments
1583	82	F-082	F attached to C2(sp ³)	atom-centred fragments

1584	83	F-083	F attached to C3(sp3)	atom-centred fragments	
1585	84	F-084	F attached to C1(sp2)	atom-centred fragments	
1586	85	F-085	F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	atom-centred fragments	
1587	86	Cl-086	Cl attached to C1(sp3)	atom-centred fragments	
1588	87	Cl-087	Cl attached to C2(sp3)	atom-centred fragments	
1589	88	Cl-088	Cl attached to C3(sp3)	atom-centred fragments	
1590	89	Cl-089	Cl attached to C1(sp2)	atom-centred fragments	
1591	90	Cl-090	Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	atom-centred fragments	
1592	91	Br-091	Br attached to C1(sp3)	atom-centred fragments	
1593	92	Br-092	Br attached to C2(sp3)	atom-centred fragments	
1594	93	Br-093	Br attached to C3(sp3)	atom-centred fragments	
1595	94	Br-094	Br attached to C1(sp2)	atom-centred fragments	
1596	95	Br-095	Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	atom-centred fragments	
1597	96	I-096	I attached to C1(sp3)	atom-centred fragments	
1598	97	I-097	I attached to C2(sp3)	atom-centred fragments	
1599	98	I-098	I attached to C3(sp3)	atom-centred fragments	
1600	99	I-099	I attached to C1(sp2)	atom-centred fragments	
1601	100	I-100	I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	atom-centred fragments	

1602	101	F-101	fluoride ion	atom-centred fragments
1603	102	Cl-102	chloride ion	atom-centred fragments
1604	103	Br-103	bromide ion	atom-centred fragments
1605	104	I-104	iodide ion	atom-centred fragments
1606	105	U-105	undefined	atom-centred fragments
1607	106	S-106	R-SH	atom-centred fragments
1608	107	S-107	R2S / RS-SR	atom-centred fragments
1609	108	S-108	R=S	atom-centred fragments
1610	109	S-109	R-SO-R	atom-centred fragments
1611	110	S-110	R-SO2-R	atom-centred fragments
1612	111	Si-111	>Si<	atom-centred fragments
1613	112	B-112	>B- as in boranes	atom-centred fragments
1614	113	U-113	undefined	atom-centred fragments
1615	114	U-114	undefined	atom-centred fragments
1616	115	P-115	P ylids	atom-centred fragments
1617	116	P-116	R3-P=X	atom-centred fragments
1618	117	P-117	X3-P=X (phosphate)	atom-centred fragments
1619	118	P-118	PX3 (phosphite)	atom-centred fragments

1620	119	P-119	PR3 (phosphine)	atom-centred fragments
1621	120	P-120	C-P(X)2=X (phosphonate)	atom-centred fragments
1622	1	qpmax	maximum positive charge	charge descriptors
1623	2	qnmax	maximum negative charge	charge descriptors
1624	3	Qpos	total positive charge	charge descriptors
1625	4	Qneg	total negative charge	charge descriptors
1626	5	Qtot	total absolute charge (electronic charge index - ECI)	charge descriptors
1627	6	Qmean	mean absolute charge (charge polarization)	charge descriptors
1628	7	Q2	total squared charge	charge descriptors
1629	8	RPCG	relative positive charge	charge descriptors
1630	9	RNCG	relative negative charge	charge descriptors
1631	10	SPP	submolecular polarity parameter	charge descriptors
1632	11	TE1	topological electronic descriptor	charge descriptors
1633	12	TE2	topological electronic descriptor (bond restricted)	charge descriptors
1634	13	PCWTe	partial charge weighted topological electronic descriptor	charge descriptors
1635	14	LDI	local dipole index	charge descriptors
1636	1	Ui	unsaturation index	molecular properties
1637	2	Hy	hydrophilic factor	molecular properties

1638	3	AMR	Ghose-Crippen molar refractivity	molecular properties
1639	4	TPSA(NO)	topological polar surface area using N,O polar contributions	molecular properties
1640	5	TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions	molecular properties
1641	6	MLOGP	Moriguchi octanol-water partition coeff. (logP)	molecular properties
1642	7	MLOGP2	Squared Moriguchi octanol-water partition coeff. (logP ²)	molecular properties
1643	8	ALOGP	Ghose-Crippen octanol-water partition coeff. (logP)	molecular properties
1644	9	ALOGP2	Squared Ghose-Crippen octanol-water partition coeff. (logP ²)	molecular properties
1645	10	LAI	Lipinski Alert index	molecular properties
1646	11	GVWAI-80	Ghose-Viswanadhan-Wendoloski drug-like index at 80%	molecular properties
1647	12	GVWAI-50	Ghose-Viswanadhan-Wendoloski drug-like index at 50%	molecular properties
1648	13	Inflammat-80	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80%	molecular properties
1649	14	Inflammat-50	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50%	molecular properties
1650	15	Depressant-80	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80%	molecular properties
1651	16	Depressant-50	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50%	molecular properties
1652	17	Psychotic-80	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80%	molecular properties
1653	18	Psychotic-50	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50%	molecular properties
1654	19	Hypertens-80	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80%	molecular properties
1655	20	Hypertens-50	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50%	molecular properties

1656	21	Hypnotic-80	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80%	molecular properties
1657	22	Hypnotic-50	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50%	molecular properties
1658	23	Neoplastic-80	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80%	molecular properties
1659	24	Neoplastic-50	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50%	molecular properties
1660	25	Infective-80	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80%	molecular properties
1661	26	Infective-50	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50%	molecular properties
1662	27	BLTF96	Verhaar model of Fish base-line toxicity from MLOGP (mmol/l)	molecular properties
1663	28	BLTD48	Verhaar model of Daphnia base-line toxicity from MLOGP (mmol/l)	molecular properties
1664	29	BLTA96	Verhaar model of Algae base-line toxicity from MLOGP (mmol/l)	molecular properties
1665	1	B01[C-C]	presence/absence of C - C at topological distance 01	2D binary fingerprints
1666	2	B01[C-N]	presence/absence of C - N at topological distance 01	2D binary fingerprints
1667	3	B01[C-O]	presence/absence of C - O at topological distance 01	2D binary fingerprints
1668	4	B01[C-S]	presence/absence of C - S at topological distance 01	2D binary fingerprints
1669	5	B01[C-P]	presence/absence of C - P at topological distance 01	2D binary fingerprints
1670	6	B01[C-F]	presence/absence of C - F at topological distance 01	2D binary fingerprints
1671	7	B01[C-Cl]	presence/absence of C - Cl at topological distance 01	2D binary fingerprints
1672	8	B01[C-Br]	presence/absence of C - Br at topological distance 01	2D binary fingerprints
1673	9	B01[C-I]	presence/absence of C - I at topological distance 01	2D binary fingerprints

1674	10	B01[C-B]	presence/absence of C - B at topological distance 01	2D binary fingerprints
1675	11	B01[C-Si]	presence/absence of C - Si at topological distance 01	2D binary fingerprints
1676	12	B01[C-X]	presence/absence of C - X at topological distance 01	2D binary fingerprints
1677	13	B01[N-N]	presence/absence of N - N at topological distance 01	2D binary fingerprints
1678	14	B01[N-O]	presence/absence of N - O at topological distance 01	2D binary fingerprints
1679	15	B01[N-S]	presence/absence of N - S at topological distance 01	2D binary fingerprints
1680	16	B01[N-P]	presence/absence of N - P at topological distance 01	2D binary fingerprints
1681	17	B01[N-F]	presence/absence of N - F at topological distance 01	2D binary fingerprints
1682	18	B01[N-Cl]	presence/absence of N - Cl at topological distance 01	2D binary fingerprints
1683	19	B01[N-Br]	presence/absence of N - Br at topological distance 01	2D binary fingerprints
1684	20	B01[N-I]	presence/absence of N - I at topological distance 01	2D binary fingerprints
1685	21	B01[N-B]	presence/absence of N - B at topological distance 01	2D binary fingerprints
1686	22	B01[N-Si]	presence/absence of N - Si at topological distance 01	2D binary fingerprints
1687	23	B01[N-X]	presence/absence of N - X at topological distance 01	2D binary fingerprints
1688	24	B01[O-O]	presence/absence of O - O at topological distance 01	2D binary fingerprints
1689	25	B01[O-S]	presence/absence of O - S at topological distance 01	2D binary fingerprints
1690	26	B01[O-P]	presence/absence of O - P at topological distance 01	2D binary fingerprints
1691	27	B01[O-F]	presence/absence of O - F at topological distance 01	2D binary fingerprints

1692	28	B01[O-Cl]	presence/absence of O - Cl at topological distance 01	2D binary fingerprints
1693	29	B01[O-Br]	presence/absence of O - Br at topological distance 01	2D binary fingerprints
1694	30	B01[O-I]	presence/absence of O - I at topological distance 01	2D binary fingerprints
1695	31	B01[O-B]	presence/absence of O - B at topological distance 01	2D binary fingerprints
1696	32	B01[O-Si]	presence/absence of O - Si at topological distance 01	2D binary fingerprints
1697	33	B01[O-X]	presence/absence of O - X at topological distance 01	2D binary fingerprints
1698	34	B01[S-S]	presence/absence of S - S at topological distance 01	2D binary fingerprints
1699	35	B01[S-P]	presence/absence of S - P at topological distance 01	2D binary fingerprints
1700	36	B01[S-F]	presence/absence of S - F at topological distance 01	2D binary fingerprints
1701	37	B01[S-Cl]	presence/absence of S - Cl at topological distance 01	2D binary fingerprints
1702	38	B01[S-Br]	presence/absence of S - Br at topological distance 01	2D binary fingerprints
1703	39	B01[S-I]	presence/absence of S - I at topological distance 01	2D binary fingerprints
1704	40	B01[S-B]	presence/absence of S - B at topological distance 01	2D binary fingerprints
1705	41	B01[S-Si]	presence/absence of S - Si at topological distance 01	2D binary fingerprints
1706	42	B01[S-X]	presence/absence of S - X at topological distance 01	2D binary fingerprints
1707	43	B01[P-P]	presence/absence of P - P at topological distance 01	2D binary fingerprints
1708	44	B01[P-F]	presence/absence of P - F at topological distance 01	2D binary fingerprints
1709	45	B01[P-Cl]	presence/absence of P - Cl at topological distance 01	2D binary fingerprints

1710	46	B01[P-Br]	presence/absence of P - Br at topological distance 01	2D binary fingerprints
1711	47	B01[P-I]	presence/absence of P - I at topological distance 01	2D binary fingerprints
1712	48	B01[P-B]	presence/absence of P - B at topological distance 01	2D binary fingerprints
1713	49	B01[P-Si]	presence/absence of P - Si at topological distance 01	2D binary fingerprints
1714	50	B01[P-X]	presence/absence of P - X at topological distance 01	2D binary fingerprints
1715	51	B01[F-F]	presence/absence of F - F at topological distance 01	2D binary fingerprints
1716	52	B01[F-Cl]	presence/absence of F - Cl at topological distance 01	2D binary fingerprints
1717	53	B01[F-Br]	presence/absence of F - Br at topological distance 01	2D binary fingerprints
1718	54	B01[F-I]	presence/absence of F - I at topological distance 01	2D binary fingerprints
1719	55	B01[F-B]	presence/absence of F - B at topological distance 01	2D binary fingerprints
1720	56	B01[F-Si]	presence/absence of F - Si at topological distance 01	2D binary fingerprints
1721	57	B01[F-X]	presence/absence of F - X at topological distance 01	2D binary fingerprints
1722	58	B01[Cl-Cl]	presence/absence of Cl - Cl at topological distance 01	2D binary fingerprints
1723	59	B01[Cl-Br]	presence/absence of Cl - Br at topological distance 01	2D binary fingerprints
1724	60	B01[Cl-I]	presence/absence of Cl - I at topological distance 01	2D binary fingerprints
1725	61	B01[Cl-B]	presence/absence of Cl - B at topological distance 01	2D binary fingerprints
1726	62	B01[Cl-Si]	presence/absence of Cl - Si at topological distance 01	2D binary fingerprints
1727	63	B01[Cl-X]	presence/absence of Cl - X at topological distance 01	2D binary fingerprints

1728	64	B01[Br-Br]	presence/absence of Br - Br at topological distance 01	2D binary fingerprints
1729	65	B01[Br-I]	presence/absence of Br - I at topological distance 01	2D binary fingerprints
1730	66	B01[Br-B]	presence/absence of Br - B at topological distance 01	2D binary fingerprints
1731	67	B01[Br-Si]	presence/absence of Br - Si at topological distance 01	2D binary fingerprints
1732	68	B01[Br-X]	presence/absence of Br - X at topological distance 01	2D binary fingerprints
1733	69	B01[I-I]	presence/absence of I - I at topological distance 01	2D binary fingerprints
1734	70	B01[I-B]	presence/absence of I - B at topological distance 01	2D binary fingerprints
1735	71	B01[I-Si]	presence/absence of I - Si at topological distance 01	2D binary fingerprints
1736	72	B01[I-X]	presence/absence of I - X at topological distance 01	2D binary fingerprints
1737	73	B01[B-B]	presence/absence of B - B at topological distance 01	2D binary fingerprints
1738	74	B01[B-Si]	presence/absence of B - Si at topological distance 01	2D binary fingerprints
1739	75	B01[B-X]	presence/absence of B - X at topological distance 01	2D binary fingerprints
1740	76	B01[Si-Si]	presence/absence of Si - Si at topological distance 01	2D binary fingerprints
1741	77	B01[Si-X]	presence/absence of Si - X at topological distance 01	2D binary fingerprints
1742	78	B01[X-X]	presence/absence of X - X at topological distance 01	2D binary fingerprints
1743	79	B02[C-C]	presence/absence of C - C at topological distance 02	2D binary fingerprints
1744	80	B02[C-N]	presence/absence of C - N at topological distance 02	2D binary fingerprints
1745	81	B02[C-O]	presence/absence of C - O at topological distance 02	2D binary fingerprints

1746	82	B02[C-S]	presence/absence of C - S at topological distance 02	2D binary fingerprints
1747	83	B02[C-P]	presence/absence of C - P at topological distance 02	2D binary fingerprints
1748	84	B02[C-F]	presence/absence of C - F at topological distance 02	2D binary fingerprints
1749	85	B02[C-Cl]	presence/absence of C - Cl at topological distance 02	2D binary fingerprints
1750	86	B02[C-Br]	presence/absence of C - Br at topological distance 02	2D binary fingerprints
1751	87	B02[C-I]	presence/absence of C - I at topological distance 02	2D binary fingerprints
1752	88	B02[C-B]	presence/absence of C - B at topological distance 02	2D binary fingerprints
1753	89	B02[C-Si]	presence/absence of C - Si at topological distance 02	2D binary fingerprints
1754	90	B02[C-X]	presence/absence of C - X at topological distance 02	2D binary fingerprints
1755	91	B02[N-N]	presence/absence of N - N at topological distance 02	2D binary fingerprints
1756	92	B02[N-O]	presence/absence of N - O at topological distance 02	2D binary fingerprints
1757	93	B02[N-S]	presence/absence of N - S at topological distance 02	2D binary fingerprints
1758	94	B02[N-P]	presence/absence of N - P at topological distance 02	2D binary fingerprints
1759	95	B02[N-F]	presence/absence of N - F at topological distance 02	2D binary fingerprints
1760	96	B02[N-Cl]	presence/absence of N - Cl at topological distance 02	2D binary fingerprints
1761	97	B02[N-Br]	presence/absence of N - Br at topological distance 02	2D binary fingerprints
1762	98	B02[N-I]	presence/absence of N - I at topological distance 02	2D binary fingerprints
1763	99	B02[N-B]	presence/absence of N - B at topological distance 02	2D binary fingerprints

1764	100	B02[N-Si]	presence/absence of N - Si at topological distance 02	2D binary fingerprints
1765	101	B02[N-X]	presence/absence of N - X at topological distance 02	2D binary fingerprints
1766	102	B02[O-O]	presence/absence of O - O at topological distance 02	2D binary fingerprints
1767	103	B02[O-S]	presence/absence of O - S at topological distance 02	2D binary fingerprints
1768	104	B02[O-P]	presence/absence of O - P at topological distance 02	2D binary fingerprints
1769	105	B02[O-F]	presence/absence of O - F at topological distance 02	2D binary fingerprints
1770	106	B02[O-Cl]	presence/absence of O - Cl at topological distance 02	2D binary fingerprints
1771	107	B02[O-Br]	presence/absence of O - Br at topological distance 02	2D binary fingerprints
1772	108	B02[O-I]	presence/absence of O - I at topological distance 02	2D binary fingerprints
1773	109	B02[O-B]	presence/absence of O - B at topological distance 02	2D binary fingerprints
1774	110	B02[O-Si]	presence/absence of O - Si at topological distance 02	2D binary fingerprints
1775	111	B02[O-X]	presence/absence of O - X at topological distance 02	2D binary fingerprints
1776	112	B02[S-S]	presence/absence of S - S at topological distance 02	2D binary fingerprints
1777	113	B02[S-P]	presence/absence of S - P at topological distance 02	2D binary fingerprints
1778	114	B02[S-F]	presence/absence of S - F at topological distance 02	2D binary fingerprints
1779	115	B02[S-Cl]	presence/absence of S - Cl at topological distance 02	2D binary fingerprints
1780	116	B02[S-Br]	presence/absence of S - Br at topological distance 02	2D binary fingerprints
1781	117	B02[S-I]	presence/absence of S - I at topological distance 02	2D binary fingerprints

1782	118	B02[S-B]	presence/absence of S - B at topological distance 02	2D binary fingerprints
1783	119	B02[S-Si]	presence/absence of S - Si at topological distance 02	2D binary fingerprints
1784	120	B02[S-X]	presence/absence of S - X at topological distance 02	2D binary fingerprints
1785	121	B02[P-P]	presence/absence of P - P at topological distance 02	2D binary fingerprints
1786	122	B02[P-F]	presence/absence of P - F at topological distance 02	2D binary fingerprints
1787	123	B02[P-Cl]	presence/absence of P - Cl at topological distance 02	2D binary fingerprints
1788	124	B02[P-Br]	presence/absence of P - Br at topological distance 02	2D binary fingerprints
1789	125	B02[P-I]	presence/absence of P - I at topological distance 02	2D binary fingerprints
1790	126	B02[P-B]	presence/absence of P - B at topological distance 02	2D binary fingerprints
1791	127	B02[P-Si]	presence/absence of P - Si at topological distance 02	2D binary fingerprints
1792	128	B02[P-X]	presence/absence of P - X at topological distance 02	2D binary fingerprints
1793	129	B02[F-F]	presence/absence of F - F at topological distance 02	2D binary fingerprints
1794	130	B02[F-Cl]	presence/absence of F - Cl at topological distance 02	2D binary fingerprints
1795	131	B02[F-Br]	presence/absence of F - Br at topological distance 02	2D binary fingerprints
1796	132	B02[F-I]	presence/absence of F - I at topological distance 02	2D binary fingerprints
1797	133	B02[F-B]	presence/absence of F - B at topological distance 02	2D binary fingerprints
1798	134	B02[F-Si]	presence/absence of F - Si at topological distance 02	2D binary fingerprints
1799	135	B02[F-X]	presence/absence of F - X at topological distance 02	2D binary fingerprints

1800	136	B02[Cl-Cl]	presence/absence of Cl - Cl at topological distance 02	2D binary fingerprints
1801	137	B02[Cl-Br]	presence/absence of Cl - Br at topological distance 02	2D binary fingerprints
1802	138	B02[Cl-I]	presence/absence of Cl - I at topological distance 02	2D binary fingerprints
1803	139	B02[Cl-B]	presence/absence of Cl - B at topological distance 02	2D binary fingerprints
1804	140	B02[Cl-Si]	presence/absence of Cl - Si at topological distance 02	2D binary fingerprints
1805	141	B02[Cl-X]	presence/absence of Cl - X at topological distance 02	2D binary fingerprints
1806	142	B02[Br-Br]	presence/absence of Br - Br at topological distance 02	2D binary fingerprints
1807	143	B02[Br-I]	presence/absence of Br - I at topological distance 02	2D binary fingerprints
1808	144	B02[Br-B]	presence/absence of Br - B at topological distance 02	2D binary fingerprints
1809	145	B02[Br-Si]	presence/absence of Br - Si at topological distance 02	2D binary fingerprints
1810	146	B02[Br-X]	presence/absence of Br - X at topological distance 02	2D binary fingerprints
1811	147	B02[I-I]	presence/absence of I - I at topological distance 02	2D binary fingerprints
1812	148	B02[I-B]	presence/absence of I - B at topological distance 02	2D binary fingerprints
1813	149	B02[I-Si]	presence/absence of I - Si at topological distance 02	2D binary fingerprints
1814	150	B02[I-X]	presence/absence of I - X at topological distance 02	2D binary fingerprints
1815	151	B02[B-B]	presence/absence of B - B at topological distance 02	2D binary fingerprints
1816	152	B02[B-Si]	presence/absence of B - Si at topological distance 02	2D binary fingerprints
1817	153	B02[B-X]	presence/absence of B - X at topological distance 02	2D binary fingerprints

1818	154	B02[Si-Si]	presence/absence of Si - Si at topological distance 02	2D binary fingerprints
1819	155	B02[Si-X]	presence/absence of Si - X at topological distance 02	2D binary fingerprints
1820	156	B02[X-X]	presence/absence of X - X at topological distance 02	2D binary fingerprints
1821	157	B03[C-C]	presence/absence of C - C at topological distance 03	2D binary fingerprints
1822	158	B03[C-N]	presence/absence of C - N at topological distance 03	2D binary fingerprints
1823	159	B03[C-O]	presence/absence of C - O at topological distance 03	2D binary fingerprints
1824	160	B03[C-S]	presence/absence of C - S at topological distance 03	2D binary fingerprints
1825	161	B03[C-P]	presence/absence of C - P at topological distance 03	2D binary fingerprints
1826	162	B03[C-F]	presence/absence of C - F at topological distance 03	2D binary fingerprints
1827	163	B03[C-Cl]	presence/absence of C - Cl at topological distance 03	2D binary fingerprints
1828	164	B03[C-Br]	presence/absence of C - Br at topological distance 03	2D binary fingerprints
1829	165	B03[C-I]	presence/absence of C - I at topological distance 03	2D binary fingerprints
1830	166	B03[C-B]	presence/absence of C - B at topological distance 03	2D binary fingerprints
1831	167	B03[C-Si]	presence/absence of C - Si at topological distance 03	2D binary fingerprints
1832	168	B03[C-X]	presence/absence of C - X at topological distance 03	2D binary fingerprints
1833	169	B03[N-N]	presence/absence of N - N at topological distance 03	2D binary fingerprints
1834	170	B03[N-O]	presence/absence of N - O at topological distance 03	2D binary fingerprints
1835	171	B03[N-S]	presence/absence of N - S at topological distance 03	2D binary fingerprints

1836	172	B03[N-P]	presence/absence of N - P at topological distance 03	2D binary fingerprints
1837	173	B03[N-F]	presence/absence of N - F at topological distance 03	2D binary fingerprints
1838	174	B03[N-Cl]	presence/absence of N - Cl at topological distance 03	2D binary fingerprints
1839	175	B03[N-Br]	presence/absence of N - Br at topological distance 03	2D binary fingerprints
1840	176	B03[N-I]	presence/absence of N - I at topological distance 03	2D binary fingerprints
1841	177	B03[N-B]	presence/absence of N - B at topological distance 03	2D binary fingerprints
1842	178	B03[N-Si]	presence/absence of N - Si at topological distance 03	2D binary fingerprints
1843	179	B03[N-X]	presence/absence of N - X at topological distance 03	2D binary fingerprints
1844	180	B03[O-O]	presence/absence of O - O at topological distance 03	2D binary fingerprints
1845	181	B03[O-S]	presence/absence of O - S at topological distance 03	2D binary fingerprints
1846	182	B03[O-P]	presence/absence of O - P at topological distance 03	2D binary fingerprints
1847	183	B03[O-F]	presence/absence of O - F at topological distance 03	2D binary fingerprints
1848	184	B03[O-Cl]	presence/absence of O - Cl at topological distance 03	2D binary fingerprints
1849	185	B03[O-Br]	presence/absence of O - Br at topological distance 03	2D binary fingerprints
1850	186	B03[O-I]	presence/absence of O - I at topological distance 03	2D binary fingerprints
1851	187	B03[O-B]	presence/absence of O - B at topological distance 03	2D binary fingerprints
1852	188	B03[O-Si]	presence/absence of O - Si at topological distance 03	2D binary fingerprints
1853	189	B03[O-X]	presence/absence of O - X at topological distance 03	2D binary fingerprints

1854	190	B03[S-S]	presence/absence of S - S at topological distance 03	2D binary fingerprints
1855	191	B03[S-P]	presence/absence of S - P at topological distance 03	2D binary fingerprints
1856	192	B03[S-F]	presence/absence of S - F at topological distance 03	2D binary fingerprints
1857	193	B03[S-Cl]	presence/absence of S - Cl at topological distance 03	2D binary fingerprints
1858	194	B03[S-Br]	presence/absence of S - Br at topological distance 03	2D binary fingerprints
1859	195	B03[S-I]	presence/absence of S - I at topological distance 03	2D binary fingerprints
1860	196	B03[S-B]	presence/absence of S - B at topological distance 03	2D binary fingerprints
1861	197	B03[S-Si]	presence/absence of S - Si at topological distance 03	2D binary fingerprints
1862	198	B03[S-X]	presence/absence of S - X at topological distance 03	2D binary fingerprints
1863	199	B03[P-P]	presence/absence of P - P at topological distance 03	2D binary fingerprints
1864	200	B03[P-F]	presence/absence of P - F at topological distance 03	2D binary fingerprints
1865	201	B03[P-Cl]	presence/absence of P - Cl at topological distance 03	2D binary fingerprints
1866	202	B03[P-Br]	presence/absence of P - Br at topological distance 03	2D binary fingerprints
1867	203	B03[P-I]	presence/absence of P - I at topological distance 03	2D binary fingerprints
1868	204	B03[P-B]	presence/absence of P - B at topological distance 03	2D binary fingerprints
1869	205	B03[P-Si]	presence/absence of P - Si at topological distance 03	2D binary fingerprints
1870	206	B03[P-X]	presence/absence of P - X at topological distance 03	2D binary fingerprints
1871	207	B03[F-F]	presence/absence of F - F at topological distance 03	2D binary fingerprints

1872	208	B03[F-Cl]	presence/absence of F - Cl at topological distance 03	2D binary fingerprints
1873	209	B03[F-Br]	presence/absence of F - Br at topological distance 03	2D binary fingerprints
1874	210	B03[F-I]	presence/absence of F - I at topological distance 03	2D binary fingerprints
1875	211	B03[F-B]	presence/absence of F - B at topological distance 03	2D binary fingerprints
1876	212	B03[F-Si]	presence/absence of F - Si at topological distance 03	2D binary fingerprints
1877	213	B03[F-X]	presence/absence of F - X at topological distance 03	2D binary fingerprints
1878	214	B03[Cl-Cl]	presence/absence of Cl - Cl at topological distance 03	2D binary fingerprints
1879	215	B03[Cl-Br]	presence/absence of Cl - Br at topological distance 03	2D binary fingerprints
1880	216	B03[Cl-I]	presence/absence of Cl - I at topological distance 03	2D binary fingerprints
1881	217	B03[Cl-B]	presence/absence of Cl - B at topological distance 03	2D binary fingerprints
1882	218	B03[Cl-Si]	presence/absence of Cl - Si at topological distance 03	2D binary fingerprints
1883	219	B03[Cl-X]	presence/absence of Cl - X at topological distance 03	2D binary fingerprints
1884	220	B03[Br-Br]	presence/absence of Br - Br at topological distance 03	2D binary fingerprints
1885	221	B03[Br-I]	presence/absence of Br - I at topological distance 03	2D binary fingerprints
1886	222	B03[Br-B]	presence/absence of Br - B at topological distance 03	2D binary fingerprints
1887	223	B03[Br-Si]	presence/absence of Br - Si at topological distance 03	2D binary fingerprints
1888	224	B03[Br-X]	presence/absence of Br - X at topological distance 03	2D binary fingerprints
1889	225	B03[I-I]	presence/absence of I - I at topological distance 03	2D binary fingerprints

1890	226	B03[I-B]	presence/absence of I - B at topological distance 03	2D binary fingerprints
1891	227	B03[I-Si]	presence/absence of I - Si at topological distance 03	2D binary fingerprints
1892	228	B03[I-X]	presence/absence of I - X at topological distance 03	2D binary fingerprints
1893	229	B03[B-B]	presence/absence of B - B at topological distance 03	2D binary fingerprints
1894	230	B03[B-Si]	presence/absence of B - Si at topological distance 03	2D binary fingerprints
1895	231	B03[B-X]	presence/absence of B - X at topological distance 03	2D binary fingerprints
1896	232	B03[Si-Si]	presence/absence of Si - Si at topological distance 03	2D binary fingerprints
1897	233	B03[Si-X]	presence/absence of Si - X at topological distance 03	2D binary fingerprints
1898	234	B03[X-X]	presence/absence of X - X at topological distance 03	2D binary fingerprints
1899	235	B04[C-C]	presence/absence of C - C at topological distance 04	2D binary fingerprints
1900	236	B04[C-N]	presence/absence of C - N at topological distance 04	2D binary fingerprints
1901	237	B04[C-O]	presence/absence of C - O at topological distance 04	2D binary fingerprints
1902	238	B04[C-S]	presence/absence of C - S at topological distance 04	2D binary fingerprints
1903	239	B04[C-P]	presence/absence of C - P at topological distance 04	2D binary fingerprints
1904	240	B04[C-F]	presence/absence of C - F at topological distance 04	2D binary fingerprints
1905	241	B04[C-Cl]	presence/absence of C - Cl at topological distance 04	2D binary fingerprints
1906	242	B04[C-Br]	presence/absence of C - Br at topological distance 04	2D binary fingerprints
1907	243	B04[C-I]	presence/absence of C - I at topological distance 04	2D binary fingerprints

1908	244	B04[C-B]	presence/absence of C - B at topological distance 04	2D binary fingerprints
1909	245	B04[C-Si]	presence/absence of C - Si at topological distance 04	2D binary fingerprints
1910	246	B04[C-X]	presence/absence of C - X at topological distance 04	2D binary fingerprints
1911	247	B04[N-N]	presence/absence of N - N at topological distance 04	2D binary fingerprints
1912	248	B04[N-O]	presence/absence of N - O at topological distance 04	2D binary fingerprints
1913	249	B04[N-S]	presence/absence of N - S at topological distance 04	2D binary fingerprints
1914	250	B04[N-P]	presence/absence of N - P at topological distance 04	2D binary fingerprints
1915	251	B04[N-F]	presence/absence of N - F at topological distance 04	2D binary fingerprints
1916	252	B04[N-Cl]	presence/absence of N - Cl at topological distance 04	2D binary fingerprints
1917	253	B04[N-Br]	presence/absence of N - Br at topological distance 04	2D binary fingerprints
1918	254	B04[N-I]	presence/absence of N - I at topological distance 04	2D binary fingerprints
1919	255	B04[N-B]	presence/absence of N - B at topological distance 04	2D binary fingerprints
1920	256	B04[N-Si]	presence/absence of N - Si at topological distance 04	2D binary fingerprints
1921	257	B04[N-X]	presence/absence of N - X at topological distance 04	2D binary fingerprints
1922	258	B04[O-O]	presence/absence of O - O at topological distance 04	2D binary fingerprints
1923	259	B04[O-S]	presence/absence of O - S at topological distance 04	2D binary fingerprints
1924	260	B04[O-P]	presence/absence of O - P at topological distance 04	2D binary fingerprints
1925	261	B04[O-F]	presence/absence of O - F at topological distance 04	2D binary fingerprints

1926	262	B04[O-Cl]	presence/absence of O - Cl at topological distance 04	2D binary fingerprints
1927	263	B04[O-Br]	presence/absence of O - Br at topological distance 04	2D binary fingerprints
1928	264	B04[O-I]	presence/absence of O - I at topological distance 04	2D binary fingerprints
1929	265	B04[O-B]	presence/absence of O - B at topological distance 04	2D binary fingerprints
1930	266	B04[O-Si]	presence/absence of O - Si at topological distance 04	2D binary fingerprints
1931	267	B04[O-X]	presence/absence of O - X at topological distance 04	2D binary fingerprints
1932	268	B04[S-S]	presence/absence of S - S at topological distance 04	2D binary fingerprints
1933	269	B04[S-P]	presence/absence of S - P at topological distance 04	2D binary fingerprints
1934	270	B04[S-F]	presence/absence of S - F at topological distance 04	2D binary fingerprints
1935	271	B04[S-Cl]	presence/absence of S - Cl at topological distance 04	2D binary fingerprints
1936	272	B04[S-Br]	presence/absence of S - Br at topological distance 04	2D binary fingerprints
1937	273	B04[S-I]	presence/absence of S - I at topological distance 04	2D binary fingerprints
1938	274	B04[S-B]	presence/absence of S - B at topological distance 04	2D binary fingerprints
1939	275	B04[S-Si]	presence/absence of S - Si at topological distance 04	2D binary fingerprints
1940	276	B04[S-X]	presence/absence of S - X at topological distance 04	2D binary fingerprints
1941	277	B04[P-P]	presence/absence of P - P at topological distance 04	2D binary fingerprints
1942	278	B04[P-F]	presence/absence of P - F at topological distance 04	2D binary fingerprints
1943	279	B04[P-Cl]	presence/absence of P - Cl at topological distance 04	2D binary fingerprints

1944	280	B04[P-Br]	presence/absence of P - Br at topological distance 04	2D binary fingerprints
1945	281	B04[P-I]	presence/absence of P - I at topological distance 04	2D binary fingerprints
1946	282	B04[P-B]	presence/absence of P - B at topological distance 04	2D binary fingerprints
1947	283	B04[P-Si]	presence/absence of P - Si at topological distance 04	2D binary fingerprints
1948	284	B04[P-X]	presence/absence of P - X at topological distance 04	2D binary fingerprints
1949	285	B04[F-F]	presence/absence of F - F at topological distance 04	2D binary fingerprints
1950	286	B04[F-Cl]	presence/absence of F - Cl at topological distance 04	2D binary fingerprints
1951	287	B04[F-Br]	presence/absence of F - Br at topological distance 04	2D binary fingerprints
1952	288	B04[F-I]	presence/absence of F - I at topological distance 04	2D binary fingerprints
1953	289	B04[F-B]	presence/absence of F - B at topological distance 04	2D binary fingerprints
1954	290	B04[F-Si]	presence/absence of F - Si at topological distance 04	2D binary fingerprints
1955	291	B04[F-X]	presence/absence of F - X at topological distance 04	2D binary fingerprints
1956	292	B04[Cl-Cl]	presence/absence of Cl - Cl at topological distance 04	2D binary fingerprints
1957	293	B04[Cl-Br]	presence/absence of Cl - Br at topological distance 04	2D binary fingerprints
1958	294	B04[Cl-I]	presence/absence of Cl - I at topological distance 04	2D binary fingerprints
1959	295	B04[Cl-B]	presence/absence of Cl - B at topological distance 04	2D binary fingerprints
1960	296	B04[Cl-Si]	presence/absence of Cl - Si at topological distance 04	2D binary fingerprints
1961	297	B04[Cl-X]	presence/absence of Cl - X at topological distance 04	2D binary fingerprints

1962	298	B04[Br-Br]	presence/absence of Br - Br at topological distance 04	2D binary fingerprints
1963	299	B04[Br-I]	presence/absence of Br - I at topological distance 04	2D binary fingerprints
1964	300	B04[Br-B]	presence/absence of Br - B at topological distance 04	2D binary fingerprints
1965	301	B04[Br-Si]	presence/absence of Br - Si at topological distance 04	2D binary fingerprints
1966	302	B04[Br-X]	presence/absence of Br - X at topological distance 04	2D binary fingerprints
1967	303	B04[I-I]	presence/absence of I - I at topological distance 04	2D binary fingerprints
1968	304	B04[I-B]	presence/absence of I - B at topological distance 04	2D binary fingerprints
1969	305	B04[I-Si]	presence/absence of I - Si at topological distance 04	2D binary fingerprints
1970	306	B04[I-X]	presence/absence of I - X at topological distance 04	2D binary fingerprints
1971	307	B04[B-B]	presence/absence of B - B at topological distance 04	2D binary fingerprints
1972	308	B04[B-Si]	presence/absence of B - Si at topological distance 04	2D binary fingerprints
1973	309	B04[B-X]	presence/absence of B - X at topological distance 04	2D binary fingerprints
1974	310	B04[Si-Si]	presence/absence of Si - Si at topological distance 04	2D binary fingerprints
1975	311	B04[Si-X]	presence/absence of Si - X at topological distance 04	2D binary fingerprints
1976	312	B04[X-X]	presence/absence of X - X at topological distance 04	2D binary fingerprints
1977	313	B05[C-C]	presence/absence of C - C at topological distance 05	2D binary fingerprints
1978	314	B05[C-N]	presence/absence of C - N at topological distance 05	2D binary fingerprints
1979	315	B05[C-O]	presence/absence of C - O at topological distance 05	2D binary fingerprints

1980	316	B05[C-S]	presence/absence of C - S at topological distance 05	2D binary fingerprints
1981	317	B05[C-P]	presence/absence of C - P at topological distance 05	2D binary fingerprints
1982	318	B05[C-F]	presence/absence of C - F at topological distance 05	2D binary fingerprints
1983	319	B05[C-Cl]	presence/absence of C - Cl at topological distance 05	2D binary fingerprints
1984	320	B05[C-Br]	presence/absence of C - Br at topological distance 05	2D binary fingerprints
1985	321	B05[C-I]	presence/absence of C - I at topological distance 05	2D binary fingerprints
1986	322	B05[C-B]	presence/absence of C - B at topological distance 05	2D binary fingerprints
1987	323	B05[C-Si]	presence/absence of C - Si at topological distance 05	2D binary fingerprints
1988	324	B05[C-X]	presence/absence of C - X at topological distance 05	2D binary fingerprints
1989	325	B05[N-N]	presence/absence of N - N at topological distance 05	2D binary fingerprints
1990	326	B05[N-O]	presence/absence of N - O at topological distance 05	2D binary fingerprints
1991	327	B05[N-S]	presence/absence of N - S at topological distance 05	2D binary fingerprints
1992	328	B05[N-P]	presence/absence of N - P at topological distance 05	2D binary fingerprints
1993	329	B05[N-F]	presence/absence of N - F at topological distance 05	2D binary fingerprints
1994	330	B05[N-Cl]	presence/absence of N - Cl at topological distance 05	2D binary fingerprints
1995	331	B05[N-Br]	presence/absence of N - Br at topological distance 05	2D binary fingerprints
1996	332	B05[N-I]	presence/absence of N - I at topological distance 05	2D binary fingerprints
1997	333	B05[N-B]	presence/absence of N - B at topological distance 05	2D binary fingerprints

1998	334	B05[N-Si]	presence/absence of N - Si at topological distance 05	2D binary fingerprints
1999	335	B05[N-X]	presence/absence of N - X at topological distance 05	2D binary fingerprints
2000	336	B05[O-O]	presence/absence of O - O at topological distance 05	2D binary fingerprints
2001	337	B05[O-S]	presence/absence of O - S at topological distance 05	2D binary fingerprints
2002	338	B05[O-P]	presence/absence of O - P at topological distance 05	2D binary fingerprints
2003	339	B05[O-F]	presence/absence of O - F at topological distance 05	2D binary fingerprints
2004	340	B05[O-Cl]	presence/absence of O - Cl at topological distance 05	2D binary fingerprints
2005	341	B05[O-Br]	presence/absence of O - Br at topological distance 05	2D binary fingerprints
2006	342	B05[O-I]	presence/absence of O - I at topological distance 05	2D binary fingerprints
2007	343	B05[O-B]	presence/absence of O - B at topological distance 05	2D binary fingerprints
2008	344	B05[O-Si]	presence/absence of O - Si at topological distance 05	2D binary fingerprints
2009	345	B05[O-X]	presence/absence of O - X at topological distance 05	2D binary fingerprints
2010	346	B05[S-S]	presence/absence of S - S at topological distance 05	2D binary fingerprints
2011	347	B05[S-P]	presence/absence of S - P at topological distance 05	2D binary fingerprints
2012	348	B05[S-F]	presence/absence of S - F at topological distance 05	2D binary fingerprints
2013	349	B05[S-Cl]	presence/absence of S - Cl at topological distance 05	2D binary fingerprints
2014	350	B05[S-Br]	presence/absence of S - Br at topological distance 05	2D binary fingerprints
2015	351	B05[S-I]	presence/absence of S - I at topological distance 05	2D binary fingerprints

2016	352	B05[S-B]	presence/absence of S - B at topological distance 05	2D binary fingerprints
2017	353	B05[S-Si]	presence/absence of S - Si at topological distance 05	2D binary fingerprints
2018	354	B05[S-X]	presence/absence of S - X at topological distance 05	2D binary fingerprints
2019	355	B05[P-P]	presence/absence of P - P at topological distance 05	2D binary fingerprints
2020	356	B05[P-F]	presence/absence of P - F at topological distance 05	2D binary fingerprints
2021	357	B05[P-Cl]	presence/absence of P - Cl at topological distance 05	2D binary fingerprints
2022	358	B05[P-Br]	presence/absence of P - Br at topological distance 05	2D binary fingerprints
2023	359	B05[P-I]	presence/absence of P - I at topological distance 05	2D binary fingerprints
2024	360	B05[P-B]	presence/absence of P - B at topological distance 05	2D binary fingerprints
2025	361	B05[P-Si]	presence/absence of P - Si at topological distance 05	2D binary fingerprints
2026	362	B05[P-X]	presence/absence of P - X at topological distance 05	2D binary fingerprints
2027	363	B05[F-F]	presence/absence of F - F at topological distance 05	2D binary fingerprints
2028	364	B05[F-Cl]	presence/absence of F - Cl at topological distance 05	2D binary fingerprints
2029	365	B05[F-Br]	presence/absence of F - Br at topological distance 05	2D binary fingerprints
2030	366	B05[F-I]	presence/absence of F - I at topological distance 05	2D binary fingerprints
2031	367	B05[F-B]	presence/absence of F - B at topological distance 05	2D binary fingerprints
2032	368	B05[F-Si]	presence/absence of F - Si at topological distance 05	2D binary fingerprints
2033	369	B05[F-X]	presence/absence of F - X at topological distance 05	2D binary fingerprints

2034	370	B05[Cl-Cl]	presence/absence of Cl - Cl at topological distance 05	2D binary fingerprints
2035	371	B05[Cl-Br]	presence/absence of Cl - Br at topological distance 05	2D binary fingerprints
2036	372	B05[Cl-I]	presence/absence of Cl - I at topological distance 05	2D binary fingerprints
2037	373	B05[Cl-B]	presence/absence of Cl - B at topological distance 05	2D binary fingerprints
2038	374	B05[Cl-Si]	presence/absence of Cl - Si at topological distance 05	2D binary fingerprints
2039	375	B05[Cl-X]	presence/absence of Cl - X at topological distance 05	2D binary fingerprints
2040	376	B05[Br-Br]	presence/absence of Br - Br at topological distance 05	2D binary fingerprints
2041	377	B05[Br-I]	presence/absence of Br - I at topological distance 05	2D binary fingerprints
2042	378	B05[Br-B]	presence/absence of Br - B at topological distance 05	2D binary fingerprints
2043	379	B05[Br-Si]	presence/absence of Br - Si at topological distance 05	2D binary fingerprints
2044	380	B05[Br-X]	presence/absence of Br - X at topological distance 05	2D binary fingerprints
2045	381	B05[I-I]	presence/absence of I - I at topological distance 05	2D binary fingerprints
2046	382	B05[I-B]	presence/absence of I - B at topological distance 05	2D binary fingerprints
2047	383	B05[I-Si]	presence/absence of I - Si at topological distance 05	2D binary fingerprints
2048	384	B05[I-X]	presence/absence of I - X at topological distance 05	2D binary fingerprints
2049	385	B05[B-B]	presence/absence of B - B at topological distance 05	2D binary fingerprints
2050	386	B05[B-Si]	presence/absence of B - Si at topological distance 05	2D binary fingerprints
2051	387	B05[B-X]	presence/absence of B - X at topological distance 05	2D binary fingerprints

2052	388	B05[Si-Si]	presence/absence of Si - Si at topological distance 05	2D binary fingerprints
2053	389	B05[Si-X]	presence/absence of Si - X at topological distance 05	2D binary fingerprints
2054	390	B05[X-X]	presence/absence of X - X at topological distance 05	2D binary fingerprints
2055	391	B06[C-C]	presence/absence of C - C at topological distance 06	2D binary fingerprints
2056	392	B06[C-N]	presence/absence of C - N at topological distance 06	2D binary fingerprints
2057	393	B06[C-O]	presence/absence of C - O at topological distance 06	2D binary fingerprints
2058	394	B06[C-S]	presence/absence of C - S at topological distance 06	2D binary fingerprints
2059	395	B06[C-P]	presence/absence of C - P at topological distance 06	2D binary fingerprints
2060	396	B06[C-F]	presence/absence of C - F at topological distance 06	2D binary fingerprints
2061	397	B06[C-Cl]	presence/absence of C - Cl at topological distance 06	2D binary fingerprints
2062	398	B06[C-Br]	presence/absence of C - Br at topological distance 06	2D binary fingerprints
2063	399	B06[C-I]	presence/absence of C - I at topological distance 06	2D binary fingerprints
2064	400	B06[C-B]	presence/absence of C - B at topological distance 06	2D binary fingerprints
2065	401	B06[C-Si]	presence/absence of C - Si at topological distance 06	2D binary fingerprints
2066	402	B06[C-X]	presence/absence of C - X at topological distance 06	2D binary fingerprints
2067	403	B06[N-N]	presence/absence of N - N at topological distance 06	2D binary fingerprints
2068	404	B06[N-O]	presence/absence of N - O at topological distance 06	2D binary fingerprints
2069	405	B06[N-S]	presence/absence of N - S at topological distance 06	2D binary fingerprints

2070	406	B06[N-P]	presence/absence of N - P at topological distance 06	2D binary fingerprints
2071	407	B06[N-F]	presence/absence of N - F at topological distance 06	2D binary fingerprints
2072	408	B06[N-Cl]	presence/absence of N - Cl at topological distance 06	2D binary fingerprints
2073	409	B06[N-Br]	presence/absence of N - Br at topological distance 06	2D binary fingerprints
2074	410	B06[N-I]	presence/absence of N - I at topological distance 06	2D binary fingerprints
2075	411	B06[N-B]	presence/absence of N - B at topological distance 06	2D binary fingerprints
2076	412	B06[N-Si]	presence/absence of N - Si at topological distance 06	2D binary fingerprints
2077	413	B06[N-X]	presence/absence of N - X at topological distance 06	2D binary fingerprints
2078	414	B06[O-O]	presence/absence of O - O at topological distance 06	2D binary fingerprints
2079	415	B06[O-S]	presence/absence of O - S at topological distance 06	2D binary fingerprints
2080	416	B06[O-P]	presence/absence of O - P at topological distance 06	2D binary fingerprints
2081	417	B06[O-F]	presence/absence of O - F at topological distance 06	2D binary fingerprints
2082	418	B06[O-Cl]	presence/absence of O - Cl at topological distance 06	2D binary fingerprints
2083	419	B06[O-Br]	presence/absence of O - Br at topological distance 06	2D binary fingerprints
2084	420	B06[O-I]	presence/absence of O - I at topological distance 06	2D binary fingerprints
2085	421	B06[O-B]	presence/absence of O - B at topological distance 06	2D binary fingerprints
2086	422	B06[O-Si]	presence/absence of O - Si at topological distance 06	2D binary fingerprints
2087	423	B06[O-X]	presence/absence of O - X at topological distance 06	2D binary fingerprints

2088	424	B06[S-S]	presence/absence of S - S at topological distance 06	2D binary fingerprints
2089	425	B06[S-P]	presence/absence of S - P at topological distance 06	2D binary fingerprints
2090	426	B06[S-F]	presence/absence of S - F at topological distance 06	2D binary fingerprints
2091	427	B06[S-Cl]	presence/absence of S - Cl at topological distance 06	2D binary fingerprints
2092	428	B06[S-Br]	presence/absence of S - Br at topological distance 06	2D binary fingerprints
2093	429	B06[S-I]	presence/absence of S - I at topological distance 06	2D binary fingerprints
2094	430	B06[S-B]	presence/absence of S - B at topological distance 06	2D binary fingerprints
2095	431	B06[S-Si]	presence/absence of S - Si at topological distance 06	2D binary fingerprints
2096	432	B06[S-X]	presence/absence of S - X at topological distance 06	2D binary fingerprints
2097	433	B06[P-P]	presence/absence of P - P at topological distance 06	2D binary fingerprints
2098	434	B06[P-F]	presence/absence of P - F at topological distance 06	2D binary fingerprints
2099	435	B06[P-Cl]	presence/absence of P - Cl at topological distance 06	2D binary fingerprints
2100	436	B06[P-Br]	presence/absence of P - Br at topological distance 06	2D binary fingerprints
2101	437	B06[P-I]	presence/absence of P - I at topological distance 06	2D binary fingerprints
2102	438	B06[P-B]	presence/absence of P - B at topological distance 06	2D binary fingerprints
2103	439	B06[P-Si]	presence/absence of P - Si at topological distance 06	2D binary fingerprints
2104	440	B06[P-X]	presence/absence of P - X at topological distance 06	2D binary fingerprints
2105	441	B06[F-F]	presence/absence of F - F at topological distance 06	2D binary fingerprints

2106	442	B06[F-Cl]	presence/absence of F - Cl at topological distance 06	2D binary fingerprints
2107	443	B06[F-Br]	presence/absence of F - Br at topological distance 06	2D binary fingerprints
2108	444	B06[F-I]	presence/absence of F - I at topological distance 06	2D binary fingerprints
2109	445	B06[F-B]	presence/absence of F - B at topological distance 06	2D binary fingerprints
2110	446	B06[F-Si]	presence/absence of F - Si at topological distance 06	2D binary fingerprints
2111	447	B06[F-X]	presence/absence of F - X at topological distance 06	2D binary fingerprints
2112	448	B06[Cl-Cl]	presence/absence of Cl - Cl at topological distance 06	2D binary fingerprints
2113	449	B06[Cl-Br]	presence/absence of Cl - Br at topological distance 06	2D binary fingerprints
2114	450	B06[Cl-I]	presence/absence of Cl - I at topological distance 06	2D binary fingerprints
2115	451	B06[Cl-B]	presence/absence of Cl - B at topological distance 06	2D binary fingerprints
2116	452	B06[Cl-Si]	presence/absence of Cl - Si at topological distance 06	2D binary fingerprints
2117	453	B06[Cl-X]	presence/absence of Cl - X at topological distance 06	2D binary fingerprints
2118	454	B06[Br-Br]	presence/absence of Br - Br at topological distance 06	2D binary fingerprints
2119	455	B06[Br-I]	presence/absence of Br - I at topological distance 06	2D binary fingerprints
2120	456	B06[Br-B]	presence/absence of Br - B at topological distance 06	2D binary fingerprints
2121	457	B06[Br-Si]	presence/absence of Br - Si at topological distance 06	2D binary fingerprints
2122	458	B06[Br-X]	presence/absence of Br - X at topological distance 06	2D binary fingerprints
2123	459	B06[I-I]	presence/absence of I - I at topological distance 06	2D binary fingerprints

2124	460	B06[I-B]	presence/absence of I - B at topological distance 06	2D binary fingerprints
2125	461	B06[I-Si]	presence/absence of I - Si at topological distance 06	2D binary fingerprints
2126	462	B06[I-X]	presence/absence of I - X at topological distance 06	2D binary fingerprints
2127	463	B06[B-B]	presence/absence of B - B at topological distance 06	2D binary fingerprints
2128	464	B06[B-Si]	presence/absence of B - Si at topological distance 06	2D binary fingerprints
2129	465	B06[B-X]	presence/absence of B - X at topological distance 06	2D binary fingerprints
2130	466	B06[Si-Si]	presence/absence of Si - Si at topological distance 06	2D binary fingerprints
2131	467	B06[Si-X]	presence/absence of Si - X at topological distance 06	2D binary fingerprints
2132	468	B06[X-X]	presence/absence of X - X at topological distance 06	2D binary fingerprints
2133	469	B07[C-C]	presence/absence of C - C at topological distance 07	2D binary fingerprints
2134	470	B07[C-N]	presence/absence of C - N at topological distance 07	2D binary fingerprints
2135	471	B07[C-O]	presence/absence of C - O at topological distance 07	2D binary fingerprints
2136	472	B07[C-S]	presence/absence of C - S at topological distance 07	2D binary fingerprints
2137	473	B07[C-P]	presence/absence of C - P at topological distance 07	2D binary fingerprints
2138	474	B07[C-F]	presence/absence of C - F at topological distance 07	2D binary fingerprints
2139	475	B07[C-Cl]	presence/absence of C - Cl at topological distance 07	2D binary fingerprints
2140	476	B07[C-Br]	presence/absence of C - Br at topological distance 07	2D binary fingerprints
2141	477	B07[C-I]	presence/absence of C - I at topological distance 07	2D binary fingerprints

2142	478	B07[C-B]	presence/absence of C - B at topological distance 07	2D binary fingerprints
2143	479	B07[C-Si]	presence/absence of C - Si at topological distance 07	2D binary fingerprints
2144	480	B07[C-X]	presence/absence of C - X at topological distance 07	2D binary fingerprints
2145	481	B07[N-N]	presence/absence of N - N at topological distance 07	2D binary fingerprints
2146	482	B07[N-O]	presence/absence of N - O at topological distance 07	2D binary fingerprints
2147	483	B07[N-S]	presence/absence of N - S at topological distance 07	2D binary fingerprints
2148	484	B07[N-P]	presence/absence of N - P at topological distance 07	2D binary fingerprints
2149	485	B07[N-F]	presence/absence of N - F at topological distance 07	2D binary fingerprints
2150	486	B07[N-Cl]	presence/absence of N - Cl at topological distance 07	2D binary fingerprints
2151	487	B07[N-Br]	presence/absence of N - Br at topological distance 07	2D binary fingerprints
2152	488	B07[N-I]	presence/absence of N - I at topological distance 07	2D binary fingerprints
2153	489	B07[N-B]	presence/absence of N - B at topological distance 07	2D binary fingerprints
2154	490	B07[N-Si]	presence/absence of N - Si at topological distance 07	2D binary fingerprints
2155	491	B07[N-X]	presence/absence of N - X at topological distance 07	2D binary fingerprints
2156	492	B07[O-O]	presence/absence of O - O at topological distance 07	2D binary fingerprints
2157	493	B07[O-S]	presence/absence of O - S at topological distance 07	2D binary fingerprints
2158	494	B07[O-P]	presence/absence of O - P at topological distance 07	2D binary fingerprints
2159	495	B07[O-F]	presence/absence of O - F at topological distance 07	2D binary fingerprints

2160	496	B07[O-Cl]	presence/absence of O - Cl at topological distance 07	2D binary fingerprints
2161	497	B07[O-Br]	presence/absence of O - Br at topological distance 07	2D binary fingerprints
2162	498	B07[O-I]	presence/absence of O - I at topological distance 07	2D binary fingerprints
2163	499	B07[O-B]	presence/absence of O - B at topological distance 07	2D binary fingerprints
2164	500	B07[O-Si]	presence/absence of O - Si at topological distance 07	2D binary fingerprints
2165	501	B07[O-X]	presence/absence of O - X at topological distance 07	2D binary fingerprints
2166	502	B07[S-S]	presence/absence of S - S at topological distance 07	2D binary fingerprints
2167	503	B07[S-P]	presence/absence of S - P at topological distance 07	2D binary fingerprints
2168	504	B07[S-F]	presence/absence of S - F at topological distance 07	2D binary fingerprints
2169	505	B07[S-Cl]	presence/absence of S - Cl at topological distance 07	2D binary fingerprints
2170	506	B07[S-Br]	presence/absence of S - Br at topological distance 07	2D binary fingerprints
2171	507	B07[S-I]	presence/absence of S - I at topological distance 07	2D binary fingerprints
2172	508	B07[S-B]	presence/absence of S - B at topological distance 07	2D binary fingerprints
2173	509	B07[S-Si]	presence/absence of S - Si at topological distance 07	2D binary fingerprints
2174	510	B07[S-X]	presence/absence of S - X at topological distance 07	2D binary fingerprints
2175	511	B07[P-P]	presence/absence of P - P at topological distance 07	2D binary fingerprints
2176	512	B07[P-F]	presence/absence of P - F at topological distance 07	2D binary fingerprints
2177	513	B07[P-Cl]	presence/absence of P - Cl at topological distance 07	2D binary fingerprints

2178	514	B07[P-Br]	presence/absence of P - Br at topological distance 07	2D binary fingerprints
2179	515	B07[P-I]	presence/absence of P - I at topological distance 07	2D binary fingerprints
2180	516	B07[P-B]	presence/absence of P - B at topological distance 07	2D binary fingerprints
2181	517	B07[P-Si]	presence/absence of P - Si at topological distance 07	2D binary fingerprints
2182	518	B07[P-X]	presence/absence of P - X at topological distance 07	2D binary fingerprints
2183	519	B07[F-F]	presence/absence of F - F at topological distance 07	2D binary fingerprints
2184	520	B07[F-Cl]	presence/absence of F - Cl at topological distance 07	2D binary fingerprints
2185	521	B07[F-Br]	presence/absence of F - Br at topological distance 07	2D binary fingerprints
2186	522	B07[F-I]	presence/absence of F - I at topological distance 07	2D binary fingerprints
2187	523	B07[F-B]	presence/absence of F - B at topological distance 07	2D binary fingerprints
2188	524	B07[F-Si]	presence/absence of F - Si at topological distance 07	2D binary fingerprints
2189	525	B07[F-X]	presence/absence of F - X at topological distance 07	2D binary fingerprints
2190	526	B07[Cl-Cl]	presence/absence of Cl - Cl at topological distance 07	2D binary fingerprints
2191	527	B07[Cl-Br]	presence/absence of Cl - Br at topological distance 07	2D binary fingerprints
2192	528	B07[Cl-I]	presence/absence of Cl - I at topological distance 07	2D binary fingerprints
2193	529	B07[Cl-B]	presence/absence of Cl - B at topological distance 07	2D binary fingerprints
2194	530	B07[Cl-Si]	presence/absence of Cl - Si at topological distance 07	2D binary fingerprints
2195	531	B07[Cl-X]	presence/absence of Cl - X at topological distance 07	2D binary fingerprints

2196	532	B07[Br-Br]	presence/absence of Br - Br at topological distance 07	2D binary fingerprints
2197	533	B07[Br-I]	presence/absence of Br - I at topological distance 07	2D binary fingerprints
2198	534	B07[Br-B]	presence/absence of Br - B at topological distance 07	2D binary fingerprints
2199	535	B07[Br-Si]	presence/absence of Br - Si at topological distance 07	2D binary fingerprints
2200	536	B07[Br-X]	presence/absence of Br - X at topological distance 07	2D binary fingerprints
2201	537	B07[I-I]	presence/absence of I - I at topological distance 07	2D binary fingerprints
2202	538	B07[I-B]	presence/absence of I - B at topological distance 07	2D binary fingerprints
2203	539	B07[I-Si]	presence/absence of I - Si at topological distance 07	2D binary fingerprints
2204	540	B07[I-X]	presence/absence of I - X at topological distance 07	2D binary fingerprints
2205	541	B07[B-B]	presence/absence of B - B at topological distance 07	2D binary fingerprints
2206	542	B07[B-Si]	presence/absence of B - Si at topological distance 07	2D binary fingerprints
2207	543	B07[B-X]	presence/absence of B - X at topological distance 07	2D binary fingerprints
2208	544	B07[Si-Si]	presence/absence of Si - Si at topological distance 07	2D binary fingerprints
2209	545	B07[Si-X]	presence/absence of Si - X at topological distance 07	2D binary fingerprints
2210	546	B07[X-X]	presence/absence of X - X at topological distance 07	2D binary fingerprints
2211	547	B08[C-C]	presence/absence of C - C at topological distance 08	2D binary fingerprints
2212	548	B08[C-N]	presence/absence of C - N at topological distance 08	2D binary fingerprints
2213	549	B08[C-O]	presence/absence of C - O at topological distance 08	2D binary fingerprints

2214	550	B08[C-S]	presence/absence of C - S at topological distance 08	2D binary fingerprints
2215	551	B08[C-P]	presence/absence of C - P at topological distance 08	2D binary fingerprints
2216	552	B08[C-F]	presence/absence of C - F at topological distance 08	2D binary fingerprints
2217	553	B08[C-Cl]	presence/absence of C - Cl at topological distance 08	2D binary fingerprints
2218	554	B08[C-Br]	presence/absence of C - Br at topological distance 08	2D binary fingerprints
2219	555	B08[C-I]	presence/absence of C - I at topological distance 08	2D binary fingerprints
2220	556	B08[C-B]	presence/absence of C - B at topological distance 08	2D binary fingerprints
2221	557	B08[C-Si]	presence/absence of C - Si at topological distance 08	2D binary fingerprints
2222	558	B08[C-X]	presence/absence of C - X at topological distance 08	2D binary fingerprints
2223	559	B08[N-N]	presence/absence of N - N at topological distance 08	2D binary fingerprints
2224	560	B08[N-O]	presence/absence of N - O at topological distance 08	2D binary fingerprints
2225	561	B08[N-S]	presence/absence of N - S at topological distance 08	2D binary fingerprints
2226	562	B08[N-P]	presence/absence of N - P at topological distance 08	2D binary fingerprints
2227	563	B08[N-F]	presence/absence of N - F at topological distance 08	2D binary fingerprints
2228	564	B08[N-Cl]	presence/absence of N - Cl at topological distance 08	2D binary fingerprints
2229	565	B08[N-Br]	presence/absence of N - Br at topological distance 08	2D binary fingerprints
2230	566	B08[N-I]	presence/absence of N - I at topological distance 08	2D binary fingerprints
2231	567	B08[N-B]	presence/absence of N - B at topological distance 08	2D binary fingerprints

2232	568	B08[N-Si]	presence/absence of N - Si at topological distance 08	2D binary fingerprints
2233	569	B08[N-X]	presence/absence of N - X at topological distance 08	2D binary fingerprints
2234	570	B08[O-O]	presence/absence of O - O at topological distance 08	2D binary fingerprints
2235	571	B08[O-S]	presence/absence of O - S at topological distance 08	2D binary fingerprints
2236	572	B08[O-P]	presence/absence of O - P at topological distance 08	2D binary fingerprints
2237	573	B08[O-F]	presence/absence of O - F at topological distance 08	2D binary fingerprints
2238	574	B08[O-Cl]	presence/absence of O - Cl at topological distance 08	2D binary fingerprints
2239	575	B08[O-Br]	presence/absence of O - Br at topological distance 08	2D binary fingerprints
2240	576	B08[O-I]	presence/absence of O - I at topological distance 08	2D binary fingerprints
2241	577	B08[O-B]	presence/absence of O - B at topological distance 08	2D binary fingerprints
2242	578	B08[O-Si]	presence/absence of O - Si at topological distance 08	2D binary fingerprints
2243	579	B08[O-X]	presence/absence of O - X at topological distance 08	2D binary fingerprints
2244	580	B08[S-S]	presence/absence of S - S at topological distance 08	2D binary fingerprints
2245	581	B08[S-P]	presence/absence of S - P at topological distance 08	2D binary fingerprints
2246	582	B08[S-F]	presence/absence of S - F at topological distance 08	2D binary fingerprints
2247	583	B08[S-Cl]	presence/absence of S - Cl at topological distance 08	2D binary fingerprints
2248	584	B08[S-Br]	presence/absence of S - Br at topological distance 08	2D binary fingerprints
2249	585	B08[S-I]	presence/absence of S - I at topological distance 08	2D binary fingerprints

2250	586	B08[S-B]	presence/absence of S - B at topological distance 08	2D binary fingerprints
2251	587	B08[S-Si]	presence/absence of S - Si at topological distance 08	2D binary fingerprints
2252	588	B08[S-X]	presence/absence of S - X at topological distance 08	2D binary fingerprints
2253	589	B08[P-P]	presence/absence of P - P at topological distance 08	2D binary fingerprints
2254	590	B08[P-F]	presence/absence of P - F at topological distance 08	2D binary fingerprints
2255	591	B08[P-Cl]	presence/absence of P - Cl at topological distance 08	2D binary fingerprints
2256	592	B08[P-Br]	presence/absence of P - Br at topological distance 08	2D binary fingerprints
2257	593	B08[P-I]	presence/absence of P - I at topological distance 08	2D binary fingerprints
2258	594	B08[P-B]	presence/absence of P - B at topological distance 08	2D binary fingerprints
2259	595	B08[P-Si]	presence/absence of P - Si at topological distance 08	2D binary fingerprints
2260	596	B08[P-X]	presence/absence of P - X at topological distance 08	2D binary fingerprints
2261	597	B08[F-F]	presence/absence of F - F at topological distance 08	2D binary fingerprints
2262	598	B08[F-Cl]	presence/absence of F - Cl at topological distance 08	2D binary fingerprints
2263	599	B08[F-Br]	presence/absence of F - Br at topological distance 08	2D binary fingerprints
2264	600	B08[F-I]	presence/absence of F - I at topological distance 08	2D binary fingerprints
2265	601	B08[F-B]	presence/absence of F - B at topological distance 08	2D binary fingerprints
2266	602	B08[F-Si]	presence/absence of F - Si at topological distance 08	2D binary fingerprints
2267	603	B08[F-X]	presence/absence of F - X at topological distance 08	2D binary fingerprints

2268	604	B08[Cl-Cl]	presence/absence of Cl - Cl at topological distance 08	2D binary fingerprints
2269	605	B08[Cl-Br]	presence/absence of Cl - Br at topological distance 08	2D binary fingerprints
2270	606	B08[Cl-I]	presence/absence of Cl - I at topological distance 08	2D binary fingerprints
2271	607	B08[Cl-B]	presence/absence of Cl - B at topological distance 08	2D binary fingerprints
2272	608	B08[Cl-Si]	presence/absence of Cl - Si at topological distance 08	2D binary fingerprints
2273	609	B08[Cl-X]	presence/absence of Cl - X at topological distance 08	2D binary fingerprints
2274	610	B08[Br-Br]	presence/absence of Br - Br at topological distance 08	2D binary fingerprints
2275	611	B08[Br-I]	presence/absence of Br - I at topological distance 08	2D binary fingerprints
2276	612	B08[Br-B]	presence/absence of Br - B at topological distance 08	2D binary fingerprints
2277	613	B08[Br-Si]	presence/absence of Br - Si at topological distance 08	2D binary fingerprints
2278	614	B08[Br-X]	presence/absence of Br - X at topological distance 08	2D binary fingerprints
2279	615	B08[I-I]	presence/absence of I - I at topological distance 08	2D binary fingerprints
2280	616	B08[I-B]	presence/absence of I - B at topological distance 08	2D binary fingerprints
2281	617	B08[I-Si]	presence/absence of I - Si at topological distance 08	2D binary fingerprints
2282	618	B08[I-X]	presence/absence of I - X at topological distance 08	2D binary fingerprints
2283	619	B08[B-B]	presence/absence of B - B at topological distance 08	2D binary fingerprints
2284	620	B08[B-Si]	presence/absence of B - Si at topological distance 08	2D binary fingerprints
2285	621	B08[B-X]	presence/absence of B - X at topological distance 08	2D binary fingerprints

2286	622	B08[Si-Si]	presence/absence of Si - Si at topological distance 08	2D binary fingerprints
2287	623	B08[Si-X]	presence/absence of Si - X at topological distance 08	2D binary fingerprints
2288	624	B08[X-X]	presence/absence of X - X at topological distance 08	2D binary fingerprints
2289	625	B09[C-C]	presence/absence of C - C at topological distance 09	2D binary fingerprints
2290	626	B09[C-N]	presence/absence of C - N at topological distance 09	2D binary fingerprints
2291	627	B09[C-O]	presence/absence of C - O at topological distance 09	2D binary fingerprints
2292	628	B09[C-S]	presence/absence of C - S at topological distance 09	2D binary fingerprints
2293	629	B09[C-P]	presence/absence of C - P at topological distance 09	2D binary fingerprints
2294	630	B09[C-F]	presence/absence of C - F at topological distance 09	2D binary fingerprints
2295	631	B09[C-Cl]	presence/absence of C - Cl at topological distance 09	2D binary fingerprints
2296	632	B09[C-Br]	presence/absence of C - Br at topological distance 09	2D binary fingerprints
2297	633	B09[C-I]	presence/absence of C - I at topological distance 09	2D binary fingerprints
2298	634	B09[C-B]	presence/absence of C - B at topological distance 09	2D binary fingerprints
2299	635	B09[C-Si]	presence/absence of C - Si at topological distance 09	2D binary fingerprints
2300	636	B09[C-X]	presence/absence of C - X at topological distance 09	2D binary fingerprints
2301	637	B09[N-N]	presence/absence of N - N at topological distance 09	2D binary fingerprints
2302	638	B09[N-O]	presence/absence of N - O at topological distance 09	2D binary fingerprints
2303	639	B09[N-S]	presence/absence of N - S at topological distance 09	2D binary fingerprints

2304	640	B09[N-P]	presence/absence of N - P at topological distance 09	2D binary fingerprints
2305	641	B09[N-F]	presence/absence of N - F at topological distance 09	2D binary fingerprints
2306	642	B09[N-Cl]	presence/absence of N - Cl at topological distance 09	2D binary fingerprints
2307	643	B09[N-Br]	presence/absence of N - Br at topological distance 09	2D binary fingerprints
2308	644	B09[N-I]	presence/absence of N - I at topological distance 09	2D binary fingerprints
2309	645	B09[N-B]	presence/absence of N - B at topological distance 09	2D binary fingerprints
2310	646	B09[N-Si]	presence/absence of N - Si at topological distance 09	2D binary fingerprints
2311	647	B09[N-X]	presence/absence of N - X at topological distance 09	2D binary fingerprints
2312	648	B09[O-O]	presence/absence of O - O at topological distance 09	2D binary fingerprints
2313	649	B09[O-S]	presence/absence of O - S at topological distance 09	2D binary fingerprints
2314	650	B09[O-P]	presence/absence of O - P at topological distance 09	2D binary fingerprints
2315	651	B09[O-F]	presence/absence of O - F at topological distance 09	2D binary fingerprints
2316	652	B09[O-Cl]	presence/absence of O - Cl at topological distance 09	2D binary fingerprints
2317	653	B09[O-Br]	presence/absence of O - Br at topological distance 09	2D binary fingerprints
2318	654	B09[O-I]	presence/absence of O - I at topological distance 09	2D binary fingerprints
2319	655	B09[O-B]	presence/absence of O - B at topological distance 09	2D binary fingerprints
2320	656	B09[O-Si]	presence/absence of O - Si at topological distance 09	2D binary fingerprints
2321	657	B09[O-X]	presence/absence of O - X at topological distance 09	2D binary fingerprints

2322	658	B09[S-S]	presence/absence of S - S at topological distance 09	2D binary fingerprints
2323	659	B09[S-P]	presence/absence of S - P at topological distance 09	2D binary fingerprints
2324	660	B09[S-F]	presence/absence of S - F at topological distance 09	2D binary fingerprints
2325	661	B09[S-Cl]	presence/absence of S - Cl at topological distance 09	2D binary fingerprints
2326	662	B09[S-Br]	presence/absence of S - Br at topological distance 09	2D binary fingerprints
2327	663	B09[S-I]	presence/absence of S - I at topological distance 09	2D binary fingerprints
2328	664	B09[S-B]	presence/absence of S - B at topological distance 09	2D binary fingerprints
2329	665	B09[S-Si]	presence/absence of S - Si at topological distance 09	2D binary fingerprints
2330	666	B09[S-X]	presence/absence of S - X at topological distance 09	2D binary fingerprints
2331	667	B09[P-P]	presence/absence of P - P at topological distance 09	2D binary fingerprints
2332	668	B09[P-F]	presence/absence of P - F at topological distance 09	2D binary fingerprints
2333	669	B09[P-Cl]	presence/absence of P - Cl at topological distance 09	2D binary fingerprints
2334	670	B09[P-Br]	presence/absence of P - Br at topological distance 09	2D binary fingerprints
2335	671	B09[P-I]	presence/absence of P - I at topological distance 09	2D binary fingerprints
2336	672	B09[P-B]	presence/absence of P - B at topological distance 09	2D binary fingerprints
2337	673	B09[P-Si]	presence/absence of P - Si at topological distance 09	2D binary fingerprints
2338	674	B09[P-X]	presence/absence of P - X at topological distance 09	2D binary fingerprints
2339	675	B09[F-F]	presence/absence of F - F at topological distance 09	2D binary fingerprints

2340	676	B09[F-Cl]	presence/absence of F - Cl at topological distance 09	2D binary fingerprints
2341	677	B09[F-Br]	presence/absence of F - Br at topological distance 09	2D binary fingerprints
2342	678	B09[F-I]	presence/absence of F - I at topological distance 09	2D binary fingerprints
2343	679	B09[F-B]	presence/absence of F - B at topological distance 09	2D binary fingerprints
2344	680	B09[F-Si]	presence/absence of F - Si at topological distance 09	2D binary fingerprints
2345	681	B09[F-X]	presence/absence of F - X at topological distance 09	2D binary fingerprints
2346	682	B09[Cl-Cl]	presence/absence of Cl - Cl at topological distance 09	2D binary fingerprints
2347	683	B09[Cl-Br]	presence/absence of Cl - Br at topological distance 09	2D binary fingerprints
2348	684	B09[Cl-I]	presence/absence of Cl - I at topological distance 09	2D binary fingerprints
2349	685	B09[Cl-B]	presence/absence of Cl - B at topological distance 09	2D binary fingerprints
2350	686	B09[Cl-Si]	presence/absence of Cl - Si at topological distance 09	2D binary fingerprints
2351	687	B09[Cl-X]	presence/absence of Cl - X at topological distance 09	2D binary fingerprints
2352	688	B09[Br-Br]	presence/absence of Br - Br at topological distance 09	2D binary fingerprints
2353	689	B09[Br-I]	presence/absence of Br - I at topological distance 09	2D binary fingerprints
2354	690	B09[Br-B]	presence/absence of Br - B at topological distance 09	2D binary fingerprints
2355	691	B09[Br-Si]	presence/absence of Br - Si at topological distance 09	2D binary fingerprints
2356	692	B09[Br-X]	presence/absence of Br - X at topological distance 09	2D binary fingerprints
2357	693	B09[I-I]	presence/absence of I - I at topological distance 09	2D binary fingerprints

2358	694	B09[I-B]	presence/absence of I - B at topological distance 09	2D binary fingerprints
2359	695	B09[I-Si]	presence/absence of I - Si at topological distance 09	2D binary fingerprints
2360	696	B09[I-X]	presence/absence of I - X at topological distance 09	2D binary fingerprints
2361	697	B09[B-B]	presence/absence of B - B at topological distance 09	2D binary fingerprints
2362	698	B09[B-Si]	presence/absence of B - Si at topological distance 09	2D binary fingerprints
2363	699	B09[B-X]	presence/absence of B - X at topological distance 09	2D binary fingerprints
2364	700	B09[Si-Si]	presence/absence of Si - Si at topological distance 09	2D binary fingerprints
2365	701	B09[Si-X]	presence/absence of Si - X at topological distance 09	2D binary fingerprints
2366	702	B09[X-X]	presence/absence of X - X at topological distance 09	2D binary fingerprints
2367	703	B10[C-C]	presence/absence of C - C at topological distance 10	2D binary fingerprints
2368	704	B10[C-N]	presence/absence of C - N at topological distance 10	2D binary fingerprints
2369	705	B10[C-O]	presence/absence of C - O at topological distance 10	2D binary fingerprints
2370	706	B10[C-S]	presence/absence of C - S at topological distance 10	2D binary fingerprints
2371	707	B10[C-P]	presence/absence of C - P at topological distance 10	2D binary fingerprints
2372	708	B10[C-F]	presence/absence of C - F at topological distance 10	2D binary fingerprints
2373	709	B10[C-Cl]	presence/absence of C - Cl at topological distance 10	2D binary fingerprints
2374	710	B10[C-Br]	presence/absence of C - Br at topological distance 10	2D binary fingerprints
2375	711	B10[C-I]	presence/absence of C - I at topological distance 10	2D binary fingerprints

2376	712	B10[C-B]	presence/absence of C - B at topological distance 10	2D binary fingerprints
2377	713	B10[C-Si]	presence/absence of C - Si at topological distance 10	2D binary fingerprints
2378	714	B10[C-X]	presence/absence of C - X at topological distance 10	2D binary fingerprints
2379	715	B10[N-N]	presence/absence of N - N at topological distance 10	2D binary fingerprints
2380	716	B10[N-O]	presence/absence of N - O at topological distance 10	2D binary fingerprints
2381	717	B10[N-S]	presence/absence of N - S at topological distance 10	2D binary fingerprints
2382	718	B10[N-P]	presence/absence of N - P at topological distance 10	2D binary fingerprints
2383	719	B10[N-F]	presence/absence of N - F at topological distance 10	2D binary fingerprints
2384	720	B10[N-Cl]	presence/absence of N - Cl at topological distance 10	2D binary fingerprints
2385	721	B10[N-Br]	presence/absence of N - Br at topological distance 10	2D binary fingerprints
2386	722	B10[N-I]	presence/absence of N - I at topological distance 10	2D binary fingerprints
2387	723	B10[N-B]	presence/absence of N - B at topological distance 10	2D binary fingerprints
2388	724	B10[N-Si]	presence/absence of N - Si at topological distance 10	2D binary fingerprints
2389	725	B10[N-X]	presence/absence of N - X at topological distance 10	2D binary fingerprints
2390	726	B10[O-O]	presence/absence of O - O at topological distance 10	2D binary fingerprints
2391	727	B10[O-S]	presence/absence of O - S at topological distance 10	2D binary fingerprints
2392	728	B10[O-P]	presence/absence of O - P at topological distance 10	2D binary fingerprints
2393	729	B10[O-F]	presence/absence of O - F at topological distance 10	2D binary fingerprints

2394	730	B10[O-Cl]	presence/absence of O - Cl at topological distance 10	2D binary fingerprints
2395	731	B10[O-Br]	presence/absence of O - Br at topological distance 10	2D binary fingerprints
2396	732	B10[O-I]	presence/absence of O - I at topological distance 10	2D binary fingerprints
2397	733	B10[O-B]	presence/absence of O - B at topological distance 10	2D binary fingerprints
2398	734	B10[O-Si]	presence/absence of O - Si at topological distance 10	2D binary fingerprints
2399	735	B10[O-X]	presence/absence of O - X at topological distance 10	2D binary fingerprints
2400	736	B10[S-S]	presence/absence of S - S at topological distance 10	2D binary fingerprints
2401	737	B10[S-P]	presence/absence of S - P at topological distance 10	2D binary fingerprints
2402	738	B10[S-F]	presence/absence of S - F at topological distance 10	2D binary fingerprints
2403	739	B10[S-Cl]	presence/absence of S - Cl at topological distance 10	2D binary fingerprints
2404	740	B10[S-Br]	presence/absence of S - Br at topological distance 10	2D binary fingerprints
2405	741	B10[S-I]	presence/absence of S - I at topological distance 10	2D binary fingerprints
2406	742	B10[S-B]	presence/absence of S - B at topological distance 10	2D binary fingerprints
2407	743	B10[S-Si]	presence/absence of S - Si at topological distance 10	2D binary fingerprints
2408	744	B10[S-X]	presence/absence of S - X at topological distance 10	2D binary fingerprints
2409	745	B10[P-P]	presence/absence of P - P at topological distance 10	2D binary fingerprints
2410	746	B10[P-F]	presence/absence of P - F at topological distance 10	2D binary fingerprints
2411	747	B10[P-Cl]	presence/absence of P - Cl at topological distance 10	2D binary fingerprints

2412	748	B10[P-Br]	presence/absence of P - Br at topological distance 10	2D binary fingerprints
2413	749	B10[P-I]	presence/absence of P - I at topological distance 10	2D binary fingerprints
2414	750	B10[P-B]	presence/absence of P - B at topological distance 10	2D binary fingerprints
2415	751	B10[P-Si]	presence/absence of P - Si at topological distance 10	2D binary fingerprints
2416	752	B10[P-X]	presence/absence of P - X at topological distance 10	2D binary fingerprints
2417	753	B10[F-F]	presence/absence of F - F at topological distance 10	2D binary fingerprints
2418	754	B10[F-Cl]	presence/absence of F - Cl at topological distance 10	2D binary fingerprints
2419	755	B10[F-Br]	presence/absence of F - Br at topological distance 10	2D binary fingerprints
2420	756	B10[F-I]	presence/absence of F - I at topological distance 10	2D binary fingerprints
2421	757	B10[F-B]	presence/absence of F - B at topological distance 10	2D binary fingerprints
2422	758	B10[F-Si]	presence/absence of F - Si at topological distance 10	2D binary fingerprints
2423	759	B10[F-X]	presence/absence of F - X at topological distance 10	2D binary fingerprints
2424	760	B10[Cl-Cl]	presence/absence of Cl - Cl at topological distance 10	2D binary fingerprints
2425	761	B10[Cl-Br]	presence/absence of Cl - Br at topological distance 10	2D binary fingerprints
2426	762	B10[Cl-I]	presence/absence of Cl - I at topological distance 10	2D binary fingerprints
2427	763	B10[Cl-B]	presence/absence of Cl - B at topological distance 10	2D binary fingerprints
2428	764	B10[Cl-Si]	presence/absence of Cl - Si at topological distance 10	2D binary fingerprints
2429	765	B10[Cl-X]	presence/absence of Cl - X at topological distance 10	2D binary fingerprints

2430	766	B10[Br-Br]	presence/absence of Br - Br at topological distance 10	2D binary fingerprints
2431	767	B10[Br-I]	presence/absence of Br - I at topological distance 10	2D binary fingerprints
2432	768	B10[Br-B]	presence/absence of Br - B at topological distance 10	2D binary fingerprints
2433	769	B10[Br-Si]	presence/absence of Br - Si at topological distance 10	2D binary fingerprints
2434	770	B10[Br-X]	presence/absence of Br - X at topological distance 10	2D binary fingerprints
2435	771	B10[I-I]	presence/absence of I - I at topological distance 10	2D binary fingerprints
2436	772	B10[I-B]	presence/absence of I - B at topological distance 10	2D binary fingerprints
2437	773	B10[I-Si]	presence/absence of I - Si at topological distance 10	2D binary fingerprints
2438	774	B10[I-X]	presence/absence of I - X at topological distance 10	2D binary fingerprints
2439	775	B10[B-B]	presence/absence of B - B at topological distance 10	2D binary fingerprints
2440	776	B10[B-Si]	presence/absence of B - Si at topological distance 10	2D binary fingerprints
2441	777	B10[B-X]	presence/absence of B - X at topological distance 10	2D binary fingerprints
2442	778	B10[Si-Si]	presence/absence of Si - Si at topological distance 10	2D binary fingerprints
2443	779	B10[Si-X]	presence/absence of Si - X at topological distance 10	2D binary fingerprints
2444	780	B10[X-X]	presence/absence of X - X at topological distance 10	2D binary fingerprints
2445	1	F01[C-C]	frequency of C - C at topological distance 01	2D frequency fingerprints
2446	2	F01[C-N]	frequency of C - N at topological distance 01	2D frequency fingerprints
2447	3	F01[C-O]	frequency of C - O at topological distance 01	2D frequency fingerprints

2448	4	F01[C-S]	frequency of C - S at topological distance 01	2D frequency fingerprints
2449	5	F01[C-P]	frequency of C - P at topological distance 01	2D frequency fingerprints
2450	6	F01[C-F]	frequency of C - F at topological distance 01	2D frequency fingerprints
2451	7	F01[C-Cl]	frequency of C - Cl at topological distance 01	2D frequency fingerprints
2452	8	F01[C-Br]	frequency of C - Br at topological distance 01	2D frequency fingerprints
2453	9	F01[C-I]	frequency of C - I at topological distance 01	2D frequency fingerprints
2454	10	F01[C-B]	frequency of C - B at topological distance 01	2D frequency fingerprints
2455	11	F01[C-Si]	frequency of C - Si at topological distance 01	2D frequency fingerprints
2456	12	F01[C-X]	frequency of C - X at topological distance 01	2D frequency fingerprints
2457	13	F01[N-N]	frequency of N - N at topological distance 01	2D frequency fingerprints
2458	14	F01[N-O]	frequency of N - O at topological distance 01	2D frequency fingerprints
2459	15	F01[N-S]	frequency of N - S at topological distance 01	2D frequency fingerprints
2460	16	F01[N-P]	frequency of N - P at topological distance 01	2D frequency fingerprints
2461	17	F01[N-F]	frequency of N - F at topological distance 01	2D frequency fingerprints
2462	18	F01[N-Cl]	frequency of N - Cl at topological distance 01	2D frequency fingerprints
2463	19	F01[N-Br]	frequency of N - Br at topological distance 01	2D frequency fingerprints
2464	20	F01[N-I]	frequency of N - I at topological distance 01	2D frequency fingerprints
2465	21	F01[N-B]	frequency of N - B at topological distance 01	2D frequency fingerprints

2466	22	F01[N-Si]	frequency of N - Si at topological distance 01	2D frequency fingerprints
2467	23	F01[N-X]	frequency of N - X at topological distance 01	2D frequency fingerprints
2468	24	F01[O-O]	frequency of O - O at topological distance 01	2D frequency fingerprints
2469	25	F01[O-S]	frequency of O - S at topological distance 01	2D frequency fingerprints
2470	26	F01[O-P]	frequency of O - P at topological distance 01	2D frequency fingerprints
2471	27	F01[O-F]	frequency of O - F at topological distance 01	2D frequency fingerprints
2472	28	F01[O-Cl]	frequency of O - Cl at topological distance 01	2D frequency fingerprints
2473	29	F01[O-Br]	frequency of O - Br at topological distance 01	2D frequency fingerprints
2474	30	F01[O-I]	frequency of O - I at topological distance 01	2D frequency fingerprints
2475	31	F01[O-B]	frequency of O - B at topological distance 01	2D frequency fingerprints
2476	32	F01[O-Si]	frequency of O - Si at topological distance 01	2D frequency fingerprints
2477	33	F01[O-X]	frequency of O - X at topological distance 01	2D frequency fingerprints
2478	34	F01[S-S]	frequency of S - S at topological distance 01	2D frequency fingerprints
2479	35	F01[S-P]	frequency of S - P at topological distance 01	2D frequency fingerprints
2480	36	F01[S-F]	frequency of S - F at topological distance 01	2D frequency fingerprints
2481	37	F01[S-Cl]	frequency of S - Cl at topological distance 01	2D frequency fingerprints
2482	38	F01[S-Br]	frequency of S - Br at topological distance 01	2D frequency fingerprints
2483	39	F01[S-I]	frequency of S - I at topological distance 01	2D frequency fingerprints

2484	40	F01[S-B]	frequency of S - B at topological distance 01	2D frequency fingerprints
2485	41	F01[S-Si]	frequency of S - Si at topological distance 01	2D frequency fingerprints
2486	42	F01[S-X]	frequency of S - X at topological distance 01	2D frequency fingerprints
2487	43	F01[P-P]	frequency of P - P at topological distance 01	2D frequency fingerprints
2488	44	F01[P-F]	frequency of P - F at topological distance 01	2D frequency fingerprints
2489	45	F01[P-Cl]	frequency of P - Cl at topological distance 01	2D frequency fingerprints
2490	46	F01[P-Br]	frequency of P - Br at topological distance 01	2D frequency fingerprints
2491	47	F01[P-I]	frequency of P - I at topological distance 01	2D frequency fingerprints
2492	48	F01[P-B]	frequency of P - B at topological distance 01	2D frequency fingerprints
2493	49	F01[P-Si]	frequency of P - Si at topological distance 01	2D frequency fingerprints
2494	50	F01[P-X]	frequency of P - X at topological distance 01	2D frequency fingerprints
2495	51	F01[F-F]	frequency of F - F at topological distance 01	2D frequency fingerprints
2496	52	F01[F-Cl]	frequency of F - Cl at topological distance 01	2D frequency fingerprints
2497	53	F01[F-Br]	frequency of F - Br at topological distance 01	2D frequency fingerprints
2498	54	F01[F-I]	frequency of F - I at topological distance 01	2D frequency fingerprints
2499	55	F01[F-B]	frequency of F - B at topological distance 01	2D frequency fingerprints
2500	56	F01[F-Si]	frequency of F - Si at topological distance 01	2D frequency fingerprints
2501	57	F01[F-X]	frequency of F - X at topological distance 01	2D frequency fingerprints

2502	58	F01[Cl-Cl]	frequency of Cl - Cl at topological distance 01	2D frequency fingerprints
2503	59	F01[Cl-Br]	frequency of Cl - Br at topological distance 01	2D frequency fingerprints
2504	60	F01[Cl-I]	frequency of Cl - I at topological distance 01	2D frequency fingerprints
2505	61	F01[Cl-B]	frequency of Cl - B at topological distance 01	2D frequency fingerprints
2506	62	F01[Cl-Si]	frequency of Cl - Si at topological distance 01	2D frequency fingerprints
2507	63	F01[Cl-X]	frequency of Cl - X at topological distance 01	2D frequency fingerprints
2508	64	F01[Br-Br]	frequency of Br - Br at topological distance 01	2D frequency fingerprints
2509	65	F01[Br-I]	frequency of Br - I at topological distance 01	2D frequency fingerprints
2510	66	F01[Br-B]	frequency of Br - B at topological distance 01	2D frequency fingerprints
2511	67	F01[Br-Si]	frequency of Br - Si at topological distance 01	2D frequency fingerprints
2512	68	F01[Br-X]	frequency of Br - X at topological distance 01	2D frequency fingerprints
2513	69	F01[I-I]	frequency of I - I at topological distance 01	2D frequency fingerprints
2514	70	F01[I-B]	frequency of I - B at topological distance 01	2D frequency fingerprints
2515	71	F01[I-Si]	frequency of I - Si at topological distance 01	2D frequency fingerprints
2516	72	F01[I-X]	frequency of I - X at topological distance 01	2D frequency fingerprints
2517	73	F01[B-B]	frequency of B - B at topological distance 01	2D frequency fingerprints
2518	74	F01[B-Si]	frequency of B - Si at topological distance 01	2D frequency fingerprints
2519	75	F01[B-X]	frequency of B - X at topological distance 01	2D frequency fingerprints

2520	76	F01[Si-Si]	frequency of Si - Si at topological distance 01	2D frequency fingerprints
2521	77	F01[Si-X]	frequency of Si - X at topological distance 01	2D frequency fingerprints
2522	78	F01[X-X]	frequency of X - X at topological distance 01	2D frequency fingerprints
2523	79	F02[C-C]	frequency of C - C at topological distance 02	2D frequency fingerprints
2524	80	F02[C-N]	frequency of C - N at topological distance 02	2D frequency fingerprints
2525	81	F02[C-O]	frequency of C - O at topological distance 02	2D frequency fingerprints
2526	82	F02[C-S]	frequency of C - S at topological distance 02	2D frequency fingerprints
2527	83	F02[C-P]	frequency of C - P at topological distance 02	2D frequency fingerprints
2528	84	F02[C-F]	frequency of C - F at topological distance 02	2D frequency fingerprints
2529	85	F02[C-Cl]	frequency of C - Cl at topological distance 02	2D frequency fingerprints
2530	86	F02[C-Br]	frequency of C - Br at topological distance 02	2D frequency fingerprints
2531	87	F02[C-I]	frequency of C - I at topological distance 02	2D frequency fingerprints
2532	88	F02[C-B]	frequency of C - B at topological distance 02	2D frequency fingerprints
2533	89	F02[C-Si]	frequency of C - Si at topological distance 02	2D frequency fingerprints
2534	90	F02[C-X]	frequency of C - X at topological distance 02	2D frequency fingerprints
2535	91	F02[N-N]	frequency of N - N at topological distance 02	2D frequency fingerprints
2536	92	F02[N-O]	frequency of N - O at topological distance 02	2D frequency fingerprints
2537	93	F02[N-S]	frequency of N - S at topological distance 02	2D frequency fingerprints

2538	94	F02[N-P]	frequency of N - P at topological distance 02	2D frequency fingerprints
2539	95	F02[N-F]	frequency of N - F at topological distance 02	2D frequency fingerprints
2540	96	F02[N-Cl]	frequency of N - Cl at topological distance 02	2D frequency fingerprints
2541	97	F02[N-Br]	frequency of N - Br at topological distance 02	2D frequency fingerprints
2542	98	F02[N-I]	frequency of N - I at topological distance 02	2D frequency fingerprints
2543	99	F02[N-B]	frequency of N - B at topological distance 02	2D frequency fingerprints
2544	100	F02[N-Si]	frequency of N - Si at topological distance 02	2D frequency fingerprints
2545	101	F02[N-X]	frequency of N - X at topological distance 02	2D frequency fingerprints
2546	102	F02[O-O]	frequency of O - O at topological distance 02	2D frequency fingerprints
2547	103	F02[O-S]	frequency of O - S at topological distance 02	2D frequency fingerprints
2548	104	F02[O-P]	frequency of O - P at topological distance 02	2D frequency fingerprints
2549	105	F02[O-F]	frequency of O - F at topological distance 02	2D frequency fingerprints
2550	106	F02[O-Cl]	frequency of O - Cl at topological distance 02	2D frequency fingerprints
2551	107	F02[O-Br]	frequency of O - Br at topological distance 02	2D frequency fingerprints
2552	108	F02[O-I]	frequency of O - I at topological distance 02	2D frequency fingerprints
2553	109	F02[O-B]	frequency of O - B at topological distance 02	2D frequency fingerprints
2554	110	F02[O-Si]	frequency of O - Si at topological distance 02	2D frequency fingerprints
2555	111	F02[O-X]	frequency of O - X at topological distance 02	2D frequency fingerprints

2556	112	F02[S-S]	frequency of S - S at topological distance 02	2D frequency fingerprints
2557	113	F02[S-P]	frequency of S - P at topological distance 02	2D frequency fingerprints
2558	114	F02[S-F]	frequency of S - F at topological distance 02	2D frequency fingerprints
2559	115	F02[S-Cl]	frequency of S - Cl at topological distance 02	2D frequency fingerprints
2560	116	F02[S-Br]	frequency of S - Br at topological distance 02	2D frequency fingerprints
2561	117	F02[S-I]	frequency of S - I at topological distance 02	2D frequency fingerprints
2562	118	F02[S-B]	frequency of S - B at topological distance 02	2D frequency fingerprints
2563	119	F02[S-Si]	frequency of S - Si at topological distance 02	2D frequency fingerprints
2564	120	F02[S-X]	frequency of S - X at topological distance 02	2D frequency fingerprints
2565	121	F02[P-P]	frequency of P - P at topological distance 02	2D frequency fingerprints
2566	122	F02[P-F]	frequency of P - F at topological distance 02	2D frequency fingerprints
2567	123	F02[P-Cl]	frequency of P - Cl at topological distance 02	2D frequency fingerprints
2568	124	F02[P-Br]	frequency of P - Br at topological distance 02	2D frequency fingerprints
2569	125	F02[P-I]	frequency of P - I at topological distance 02	2D frequency fingerprints
2570	126	F02[P-B]	frequency of P - B at topological distance 02	2D frequency fingerprints
2571	127	F02[P-Si]	frequency of P - Si at topological distance 02	2D frequency fingerprints
2572	128	F02[P-X]	frequency of P - X at topological distance 02	2D frequency fingerprints
2573	129	F02[F-F]	frequency of F - F at topological distance 02	2D frequency fingerprints

2574	130	F02[F-Cl]	frequency of F - Cl at topological distance 02	2D frequency fingerprints
2575	131	F02[F-Br]	frequency of F - Br at topological distance 02	2D frequency fingerprints
2576	132	F02[F-I]	frequency of F - I at topological distance 02	2D frequency fingerprints
2577	133	F02[F-B]	frequency of F - B at topological distance 02	2D frequency fingerprints
2578	134	F02[F-Si]	frequency of F - Si at topological distance 02	2D frequency fingerprints
2579	135	F02[F-X]	frequency of F - X at topological distance 02	2D frequency fingerprints
2580	136	F02[Cl-Cl]	frequency of Cl - Cl at topological distance 02	2D frequency fingerprints
2581	137	F02[Cl-Br]	frequency of Cl - Br at topological distance 02	2D frequency fingerprints
2582	138	F02[Cl-I]	frequency of Cl - I at topological distance 02	2D frequency fingerprints
2583	139	F02[Cl-B]	frequency of Cl - B at topological distance 02	2D frequency fingerprints
2584	140	F02[Cl-Si]	frequency of Cl - Si at topological distance 02	2D frequency fingerprints
2585	141	F02[Cl-X]	frequency of Cl - X at topological distance 02	2D frequency fingerprints
2586	142	F02[Br-Br]	frequency of Br - Br at topological distance 02	2D frequency fingerprints
2587	143	F02[Br-I]	frequency of Br - I at topological distance 02	2D frequency fingerprints
2588	144	F02[Br-B]	frequency of Br - B at topological distance 02	2D frequency fingerprints
2589	145	F02[Br-Si]	frequency of Br - Si at topological distance 02	2D frequency fingerprints
2590	146	F02[Br-X]	frequency of Br - X at topological distance 02	2D frequency fingerprints
2591	147	F02[I-I]	frequency of I - I at topological distance 02	2D frequency fingerprints

2592	148	F02[I-B]	frequency of I - B at topological distance 02	2D frequency fingerprints
2593	149	F02[I-Si]	frequency of I - Si at topological distance 02	2D frequency fingerprints
2594	150	F02[I-X]	frequency of I - X at topological distance 02	2D frequency fingerprints
2595	151	F02[B-B]	frequency of B - B at topological distance 02	2D frequency fingerprints
2596	152	F02[B-Si]	frequency of B - Si at topological distance 02	2D frequency fingerprints
2597	153	F02[B-X]	frequency of B - X at topological distance 02	2D frequency fingerprints
2598	154	F02[Si-Si]	frequency of Si - Si at topological distance 02	2D frequency fingerprints
2599	155	F02[Si-X]	frequency of Si - X at topological distance 02	2D frequency fingerprints
2600	156	F02[X-X]	frequency of X - X at topological distance 02	2D frequency fingerprints
2601	157	F03[C-C]	frequency of C - C at topological distance 03	2D frequency fingerprints
2602	158	F03[C-N]	frequency of C - N at topological distance 03	2D frequency fingerprints
2603	159	F03[C-O]	frequency of C - O at topological distance 03	2D frequency fingerprints
2604	160	F03[C-S]	frequency of C - S at topological distance 03	2D frequency fingerprints
2605	161	F03[C-P]	frequency of C - P at topological distance 03	2D frequency fingerprints
2606	162	F03[C-F]	frequency of C - F at topological distance 03	2D frequency fingerprints
2607	163	F03[C-Cl]	frequency of C - Cl at topological distance 03	2D frequency fingerprints
2608	164	F03[C-Br]	frequency of C - Br at topological distance 03	2D frequency fingerprints
2609	165	F03[C-I]	frequency of C - I at topological distance 03	2D frequency fingerprints

2610	166	F03[C-B]	frequency of C - B at topological distance 03	2D frequency fingerprints
2611	167	F03[C-Si]	frequency of C - Si at topological distance 03	2D frequency fingerprints
2612	168	F03[C-X]	frequency of C - X at topological distance 03	2D frequency fingerprints
2613	169	F03[N-N]	frequency of N - N at topological distance 03	2D frequency fingerprints
2614	170	F03[N-O]	frequency of N - O at topological distance 03	2D frequency fingerprints
2615	171	F03[N-S]	frequency of N - S at topological distance 03	2D frequency fingerprints
2616	172	F03[N-P]	frequency of N - P at topological distance 03	2D frequency fingerprints
2617	173	F03[N-F]	frequency of N - F at topological distance 03	2D frequency fingerprints
2618	174	F03[N-Cl]	frequency of N - Cl at topological distance 03	2D frequency fingerprints
2619	175	F03[N-Br]	frequency of N - Br at topological distance 03	2D frequency fingerprints
2620	176	F03[N-I]	frequency of N - I at topological distance 03	2D frequency fingerprints
2621	177	F03[N-B]	frequency of N - B at topological distance 03	2D frequency fingerprints
2622	178	F03[N-Si]	frequency of N - Si at topological distance 03	2D frequency fingerprints
2623	179	F03[N-X]	frequency of N - X at topological distance 03	2D frequency fingerprints
2624	180	F03[O-O]	frequency of O - O at topological distance 03	2D frequency fingerprints
2625	181	F03[O-S]	frequency of O - S at topological distance 03	2D frequency fingerprints
2626	182	F03[O-P]	frequency of O - P at topological distance 03	2D frequency fingerprints
2627	183	F03[O-F]	frequency of O - F at topological distance 03	2D frequency fingerprints

2628	184	F03[O-Cl]	frequency of O - Cl at topological distance 03	2D frequency fingerprints
2629	185	F03[O-Br]	frequency of O - Br at topological distance 03	2D frequency fingerprints
2630	186	F03[O-I]	frequency of O - I at topological distance 03	2D frequency fingerprints
2631	187	F03[O-B]	frequency of O - B at topological distance 03	2D frequency fingerprints
2632	188	F03[O-Si]	frequency of O - Si at topological distance 03	2D frequency fingerprints
2633	189	F03[O-X]	frequency of O - X at topological distance 03	2D frequency fingerprints
2634	190	F03[S-S]	frequency of S - S at topological distance 03	2D frequency fingerprints
2635	191	F03[S-P]	frequency of S - P at topological distance 03	2D frequency fingerprints
2636	192	F03[S-F]	frequency of S - F at topological distance 03	2D frequency fingerprints
2637	193	F03[S-Cl]	frequency of S - Cl at topological distance 03	2D frequency fingerprints
2638	194	F03[S-Br]	frequency of S - Br at topological distance 03	2D frequency fingerprints
2639	195	F03[S-I]	frequency of S - I at topological distance 03	2D frequency fingerprints
2640	196	F03[S-B]	frequency of S - B at topological distance 03	2D frequency fingerprints
2641	197	F03[S-Si]	frequency of S - Si at topological distance 03	2D frequency fingerprints
2642	198	F03[S-X]	frequency of S - X at topological distance 03	2D frequency fingerprints
2643	199	F03[P-P]	frequency of P - P at topological distance 03	2D frequency fingerprints
2644	200	F03[P-F]	frequency of P - F at topological distance 03	2D frequency fingerprints
2645	201	F03[P-Cl]	frequency of P - Cl at topological distance 03	2D frequency fingerprints

2646	202	F03[P-Br]	frequency of P - Br at topological distance 03	2D frequency fingerprints
2647	203	F03[P-I]	frequency of P - I at topological distance 03	2D frequency fingerprints
2648	204	F03[P-B]	frequency of P - B at topological distance 03	2D frequency fingerprints
2649	205	F03[P-Si]	frequency of P - Si at topological distance 03	2D frequency fingerprints
2650	206	F03[P-X]	frequency of P - X at topological distance 03	2D frequency fingerprints
2651	207	F03[F-F]	frequency of F - F at topological distance 03	2D frequency fingerprints
2652	208	F03[F-Cl]	frequency of F - Cl at topological distance 03	2D frequency fingerprints
2653	209	F03[F-Br]	frequency of F - Br at topological distance 03	2D frequency fingerprints
2654	210	F03[F-I]	frequency of F - I at topological distance 03	2D frequency fingerprints
2655	211	F03[F-B]	frequency of F - B at topological distance 03	2D frequency fingerprints
2656	212	F03[F-Si]	frequency of F - Si at topological distance 03	2D frequency fingerprints
2657	213	F03[F-X]	frequency of F - X at topological distance 03	2D frequency fingerprints
2658	214	F03[Cl-Cl]	frequency of Cl - Cl at topological distance 03	2D frequency fingerprints
2659	215	F03[Cl-Br]	frequency of Cl - Br at topological distance 03	2D frequency fingerprints
2660	216	F03[Cl-I]	frequency of Cl - I at topological distance 03	2D frequency fingerprints
2661	217	F03[Cl-B]	frequency of Cl - B at topological distance 03	2D frequency fingerprints
2662	218	F03[Cl-Si]	frequency of Cl - Si at topological distance 03	2D frequency fingerprints
2663	219	F03[Cl-X]	frequency of Cl - X at topological distance 03	2D frequency fingerprints

2664	220	F03[Br-Br]	frequency of Br - Br at topological distance 03	2D frequency fingerprints
2665	221	F03[Br-I]	frequency of Br - I at topological distance 03	2D frequency fingerprints
2666	222	F03[Br-B]	frequency of Br - B at topological distance 03	2D frequency fingerprints
2667	223	F03[Br-Si]	frequency of Br - Si at topological distance 03	2D frequency fingerprints
2668	224	F03[Br-X]	frequency of Br - X at topological distance 03	2D frequency fingerprints
2669	225	F03[I-I]	frequency of I - I at topological distance 03	2D frequency fingerprints
2670	226	F03[I-B]	frequency of I - B at topological distance 03	2D frequency fingerprints
2671	227	F03[I-Si]	frequency of I - Si at topological distance 03	2D frequency fingerprints
2672	228	F03[I-X]	frequency of I - X at topological distance 03	2D frequency fingerprints
2673	229	F03[B-B]	frequency of B - B at topological distance 03	2D frequency fingerprints
2674	230	F03[B-Si]	frequency of B - Si at topological distance 03	2D frequency fingerprints
2675	231	F03[B-X]	frequency of B - X at topological distance 03	2D frequency fingerprints
2676	232	F03[Si-Si]	frequency of Si - Si at topological distance 03	2D frequency fingerprints
2677	233	F03[Si-X]	frequency of Si - X at topological distance 03	2D frequency fingerprints
2678	234	F03[X-X]	frequency of X - X at topological distance 03	2D frequency fingerprints
2679	235	F04[C-C]	frequency of C - C at topological distance 04	2D frequency fingerprints
2680	236	F04[C-N]	frequency of C - N at topological distance 04	2D frequency fingerprints
2681	237	F04[C-O]	frequency of C - O at topological distance 04	2D frequency fingerprints

2682	238	F04[C-S]	frequency of C - S at topological distance 04	2D frequency fingerprints
2683	239	F04[C-P]	frequency of C - P at topological distance 04	2D frequency fingerprints
2684	240	F04[C-F]	frequency of C - F at topological distance 04	2D frequency fingerprints
2685	241	F04[C-Cl]	frequency of C - Cl at topological distance 04	2D frequency fingerprints
2686	242	F04[C-Br]	frequency of C - Br at topological distance 04	2D frequency fingerprints
2687	243	F04[C-I]	frequency of C - I at topological distance 04	2D frequency fingerprints
2688	244	F04[C-B]	frequency of C - B at topological distance 04	2D frequency fingerprints
2689	245	F04[C-Si]	frequency of C - Si at topological distance 04	2D frequency fingerprints
2690	246	F04[C-X]	frequency of C - X at topological distance 04	2D frequency fingerprints
2691	247	F04[N-N]	frequency of N - N at topological distance 04	2D frequency fingerprints
2692	248	F04[N-O]	frequency of N - O at topological distance 04	2D frequency fingerprints
2693	249	F04[N-S]	frequency of N - S at topological distance 04	2D frequency fingerprints
2694	250	F04[N-P]	frequency of N - P at topological distance 04	2D frequency fingerprints
2695	251	F04[N-F]	frequency of N - F at topological distance 04	2D frequency fingerprints
2696	252	F04[N-Cl]	frequency of N - Cl at topological distance 04	2D frequency fingerprints
2697	253	F04[N-Br]	frequency of N - Br at topological distance 04	2D frequency fingerprints
2698	254	F04[N-I]	frequency of N - I at topological distance 04	2D frequency fingerprints
2699	255	F04[N-B]	frequency of N - B at topological distance 04	2D frequency fingerprints

2700	256	F04[N-Si]	frequency of N - Si at topological distance 04	2D frequency fingerprints
2701	257	F04[N-X]	frequency of N - X at topological distance 04	2D frequency fingerprints
2702	258	F04[O-O]	frequency of O - O at topological distance 04	2D frequency fingerprints
2703	259	F04[O-S]	frequency of O - S at topological distance 04	2D frequency fingerprints
2704	260	F04[O-P]	frequency of O - P at topological distance 04	2D frequency fingerprints
2705	261	F04[O-F]	frequency of O - F at topological distance 04	2D frequency fingerprints
2706	262	F04[O-Cl]	frequency of O - Cl at topological distance 04	2D frequency fingerprints
2707	263	F04[O-Br]	frequency of O - Br at topological distance 04	2D frequency fingerprints
2708	264	F04[O-I]	frequency of O - I at topological distance 04	2D frequency fingerprints
2709	265	F04[O-B]	frequency of O - B at topological distance 04	2D frequency fingerprints
2710	266	F04[O-Si]	frequency of O - Si at topological distance 04	2D frequency fingerprints
2711	267	F04[O-X]	frequency of O - X at topological distance 04	2D frequency fingerprints
2712	268	F04[S-S]	frequency of S - S at topological distance 04	2D frequency fingerprints
2713	269	F04[S-P]	frequency of S - P at topological distance 04	2D frequency fingerprints
2714	270	F04[S-F]	frequency of S - F at topological distance 04	2D frequency fingerprints
2715	271	F04[S-Cl]	frequency of S - Cl at topological distance 04	2D frequency fingerprints
2716	272	F04[S-Br]	frequency of S - Br at topological distance 04	2D frequency fingerprints
2717	273	F04[S-I]	frequency of S - I at topological distance 04	2D frequency fingerprints

2718	274	F04[S-B]	frequency of S - B at topological distance 04	2D frequency fingerprints
2719	275	F04[S-Si]	frequency of S - Si at topological distance 04	2D frequency fingerprints
2720	276	F04[S-X]	frequency of S - X at topological distance 04	2D frequency fingerprints
2721	277	F04[P-P]	frequency of P - P at topological distance 04	2D frequency fingerprints
2722	278	F04[P-F]	frequency of P - F at topological distance 04	2D frequency fingerprints
2723	279	F04[P-Cl]	frequency of P - Cl at topological distance 04	2D frequency fingerprints
2724	280	F04[P-Br]	frequency of P - Br at topological distance 04	2D frequency fingerprints
2725	281	F04[P-I]	frequency of P - I at topological distance 04	2D frequency fingerprints
2726	282	F04[P-B]	frequency of P - B at topological distance 04	2D frequency fingerprints
2727	283	F04[P-Si]	frequency of P - Si at topological distance 04	2D frequency fingerprints
2728	284	F04[P-X]	frequency of P - X at topological distance 04	2D frequency fingerprints
2729	285	F04[F-F]	frequency of F - F at topological distance 04	2D frequency fingerprints
2730	286	F04[F-Cl]	frequency of F - Cl at topological distance 04	2D frequency fingerprints
2731	287	F04[F-Br]	frequency of F - Br at topological distance 04	2D frequency fingerprints
2732	288	F04[F-I]	frequency of F - I at topological distance 04	2D frequency fingerprints
2733	289	F04[F-B]	frequency of F - B at topological distance 04	2D frequency fingerprints
2734	290	F04[F-Si]	frequency of F - Si at topological distance 04	2D frequency fingerprints
2735	291	F04[F-X]	frequency of F - X at topological distance 04	2D frequency fingerprints

2736	292	F04[Cl-Cl]	frequency of Cl - Cl at topological distance 04	2D frequency fingerprints
2737	293	F04[Cl-Br]	frequency of Cl - Br at topological distance 04	2D frequency fingerprints
2738	294	F04[Cl-I]	frequency of Cl - I at topological distance 04	2D frequency fingerprints
2739	295	F04[Cl-B]	frequency of Cl - B at topological distance 04	2D frequency fingerprints
2740	296	F04[Cl-Si]	frequency of Cl - Si at topological distance 04	2D frequency fingerprints
2741	297	F04[Cl-X]	frequency of Cl - X at topological distance 04	2D frequency fingerprints
2742	298	F04[Br-Br]	frequency of Br - Br at topological distance 04	2D frequency fingerprints
2743	299	F04[Br-I]	frequency of Br - I at topological distance 04	2D frequency fingerprints
2744	300	F04[Br-B]	frequency of Br - B at topological distance 04	2D frequency fingerprints
2745	301	F04[Br-Si]	frequency of Br - Si at topological distance 04	2D frequency fingerprints
2746	302	F04[Br-X]	frequency of Br - X at topological distance 04	2D frequency fingerprints
2747	303	F04[I-I]	frequency of I - I at topological distance 04	2D frequency fingerprints
2748	304	F04[I-B]	frequency of I - B at topological distance 04	2D frequency fingerprints
2749	305	F04[I-Si]	frequency of I - Si at topological distance 04	2D frequency fingerprints
2750	306	F04[I-X]	frequency of I - X at topological distance 04	2D frequency fingerprints
2751	307	F04[B-B]	frequency of B - B at topological distance 04	2D frequency fingerprints
2752	308	F04[B-Si]	frequency of B - Si at topological distance 04	2D frequency fingerprints
2753	309	F04[B-X]	frequency of B - X at topological distance 04	2D frequency fingerprints

2754	310	F04[Si-Si]	frequency of Si - Si at topological distance 04	2D frequency fingerprints
2755	311	F04[Si-X]	frequency of Si - X at topological distance 04	2D frequency fingerprints
2756	312	F04[X-X]	frequency of X - X at topological distance 04	2D frequency fingerprints
2757	313	F05[C-C]	frequency of C - C at topological distance 05	2D frequency fingerprints
2758	314	F05[C-N]	frequency of C - N at topological distance 05	2D frequency fingerprints
2759	315	F05[C-O]	frequency of C - O at topological distance 05	2D frequency fingerprints
2760	316	F05[C-S]	frequency of C - S at topological distance 05	2D frequency fingerprints
2761	317	F05[C-P]	frequency of C - P at topological distance 05	2D frequency fingerprints
2762	318	F05[C-F]	frequency of C - F at topological distance 05	2D frequency fingerprints
2763	319	F05[C-Cl]	frequency of C - Cl at topological distance 05	2D frequency fingerprints
2764	320	F05[C-Br]	frequency of C - Br at topological distance 05	2D frequency fingerprints
2765	321	F05[C-I]	frequency of C - I at topological distance 05	2D frequency fingerprints
2766	322	F05[C-B]	frequency of C - B at topological distance 05	2D frequency fingerprints
2767	323	F05[C-Si]	frequency of C - Si at topological distance 05	2D frequency fingerprints
2768	324	F05[C-X]	frequency of C - X at topological distance 05	2D frequency fingerprints
2769	325	F05[N-N]	frequency of N - N at topological distance 05	2D frequency fingerprints
2770	326	F05[N-O]	frequency of N - O at topological distance 05	2D frequency fingerprints
2771	327	F05[N-S]	frequency of N - S at topological distance 05	2D frequency fingerprints

2772	328	F05[N-P]	frequency of N - P at topological distance 05	2D frequency fingerprints
2773	329	F05[N-F]	frequency of N - F at topological distance 05	2D frequency fingerprints
2774	330	F05[N-Cl]	frequency of N - Cl at topological distance 05	2D frequency fingerprints
2775	331	F05[N-Br]	frequency of N - Br at topological distance 05	2D frequency fingerprints
2776	332	F05[N-I]	frequency of N - I at topological distance 05	2D frequency fingerprints
2777	333	F05[N-B]	frequency of N - B at topological distance 05	2D frequency fingerprints
2778	334	F05[N-Si]	frequency of N - Si at topological distance 05	2D frequency fingerprints
2779	335	F05[N-X]	frequency of N - X at topological distance 05	2D frequency fingerprints
2780	336	F05[O-O]	frequency of O - O at topological distance 05	2D frequency fingerprints
2781	337	F05[O-S]	frequency of O - S at topological distance 05	2D frequency fingerprints
2782	338	F05[O-P]	frequency of O - P at topological distance 05	2D frequency fingerprints
2783	339	F05[O-F]	frequency of O - F at topological distance 05	2D frequency fingerprints
2784	340	F05[O-Cl]	frequency of O - Cl at topological distance 05	2D frequency fingerprints
2785	341	F05[O-Br]	frequency of O - Br at topological distance 05	2D frequency fingerprints
2786	342	F05[O-I]	frequency of O - I at topological distance 05	2D frequency fingerprints
2787	343	F05[O-B]	frequency of O - B at topological distance 05	2D frequency fingerprints
2788	344	F05[O-Si]	frequency of O - Si at topological distance 05	2D frequency fingerprints
2789	345	F05[O-X]	frequency of O - X at topological distance 05	2D frequency fingerprints

2790	346	F05[S-S]	frequency of S - S at topological distance 05	2D frequency fingerprints
2791	347	F05[S-P]	frequency of S - P at topological distance 05	2D frequency fingerprints
2792	348	F05[S-F]	frequency of S - F at topological distance 05	2D frequency fingerprints
2793	349	F05[S-Cl]	frequency of S - Cl at topological distance 05	2D frequency fingerprints
2794	350	F05[S-Br]	frequency of S - Br at topological distance 05	2D frequency fingerprints
2795	351	F05[S-I]	frequency of S - I at topological distance 05	2D frequency fingerprints
2796	352	F05[S-B]	frequency of S - B at topological distance 05	2D frequency fingerprints
2797	353	F05[S-Si]	frequency of S - Si at topological distance 05	2D frequency fingerprints
2798	354	F05[S-X]	frequency of S - X at topological distance 05	2D frequency fingerprints
2799	355	F05[P-P]	frequency of P - P at topological distance 05	2D frequency fingerprints
2800	356	F05[P-F]	frequency of P - F at topological distance 05	2D frequency fingerprints
2801	357	F05[P-Cl]	frequency of P - Cl at topological distance 05	2D frequency fingerprints
2802	358	F05[P-Br]	frequency of P - Br at topological distance 05	2D frequency fingerprints
2803	359	F05[P-I]	frequency of P - I at topological distance 05	2D frequency fingerprints
2804	360	F05[P-B]	frequency of P - B at topological distance 05	2D frequency fingerprints
2805	361	F05[P-Si]	frequency of P - Si at topological distance 05	2D frequency fingerprints
2806	362	F05[P-X]	frequency of P - X at topological distance 05	2D frequency fingerprints
2807	363	F05[F-F]	frequency of F - F at topological distance 05	2D frequency fingerprints

2808	364	F05[F-Cl]	frequency of F - Cl at topological distance 05	2D frequency fingerprints
2809	365	F05[F-Br]	frequency of F - Br at topological distance 05	2D frequency fingerprints
2810	366	F05[F-I]	frequency of F - I at topological distance 05	2D frequency fingerprints
2811	367	F05[F-B]	frequency of F - B at topological distance 05	2D frequency fingerprints
2812	368	F05[F-Si]	frequency of F - Si at topological distance 05	2D frequency fingerprints
2813	369	F05[F-X]	frequency of F - X at topological distance 05	2D frequency fingerprints
2814	370	F05[Cl-Cl]	frequency of Cl - Cl at topological distance 05	2D frequency fingerprints
2815	371	F05[Cl-Br]	frequency of Cl - Br at topological distance 05	2D frequency fingerprints
2816	372	F05[Cl-I]	frequency of Cl - I at topological distance 05	2D frequency fingerprints
2817	373	F05[Cl-B]	frequency of Cl - B at topological distance 05	2D frequency fingerprints
2818	374	F05[Cl-Si]	frequency of Cl - Si at topological distance 05	2D frequency fingerprints
2819	375	F05[Cl-X]	frequency of Cl - X at topological distance 05	2D frequency fingerprints
2820	376	F05[Br-Br]	frequency of Br - Br at topological distance 05	2D frequency fingerprints
2821	377	F05[Br-I]	frequency of Br - I at topological distance 05	2D frequency fingerprints
2822	378	F05[Br-B]	frequency of Br - B at topological distance 05	2D frequency fingerprints
2823	379	F05[Br-Si]	frequency of Br - Si at topological distance 05	2D frequency fingerprints
2824	380	F05[Br-X]	frequency of Br - X at topological distance 05	2D frequency fingerprints
2825	381	F05[I-I]	frequency of I - I at topological distance 05	2D frequency fingerprints

2826	382	F05[I-B]	frequency of I - B at topological distance 05	2D frequency fingerprints
2827	383	F05[I-Si]	frequency of I - Si at topological distance 05	2D frequency fingerprints
2828	384	F05[I-X]	frequency of I - X at topological distance 05	2D frequency fingerprints
2829	385	F05[B-B]	frequency of B - B at topological distance 05	2D frequency fingerprints
2830	386	F05[B-Si]	frequency of B - Si at topological distance 05	2D frequency fingerprints
2831	387	F05[B-X]	frequency of B - X at topological distance 05	2D frequency fingerprints
2832	388	F05[Si-Si]	frequency of Si - Si at topological distance 05	2D frequency fingerprints
2833	389	F05[Si-X]	frequency of Si - X at topological distance 05	2D frequency fingerprints
2834	390	F05[X-X]	frequency of X - X at topological distance 05	2D frequency fingerprints
2835	391	F06[C-C]	frequency of C - C at topological distance 06	2D frequency fingerprints
2836	392	F06[C-N]	frequency of C - N at topological distance 06	2D frequency fingerprints
2837	393	F06[C-O]	frequency of C - O at topological distance 06	2D frequency fingerprints
2838	394	F06[C-S]	frequency of C - S at topological distance 06	2D frequency fingerprints
2839	395	F06[C-P]	frequency of C - P at topological distance 06	2D frequency fingerprints
2840	396	F06[C-F]	frequency of C - F at topological distance 06	2D frequency fingerprints
2841	397	F06[C-Cl]	frequency of C - Cl at topological distance 06	2D frequency fingerprints
2842	398	F06[C-Br]	frequency of C - Br at topological distance 06	2D frequency fingerprints
2843	399	F06[C-I]	frequency of C - I at topological distance 06	2D frequency fingerprints

2844	400	F06[C-B]	frequency of C - B at topological distance 06	2D frequency fingerprints
2845	401	F06[C-Si]	frequency of C - Si at topological distance 06	2D frequency fingerprints
2846	402	F06[C-X]	frequency of C - X at topological distance 06	2D frequency fingerprints
2847	403	F06[N-N]	frequency of N - N at topological distance 06	2D frequency fingerprints
2848	404	F06[N-O]	frequency of N - O at topological distance 06	2D frequency fingerprints
2849	405	F06[N-S]	frequency of N - S at topological distance 06	2D frequency fingerprints
2850	406	F06[N-P]	frequency of N - P at topological distance 06	2D frequency fingerprints
2851	407	F06[N-F]	frequency of N - F at topological distance 06	2D frequency fingerprints
2852	408	F06[N-Cl]	frequency of N - Cl at topological distance 06	2D frequency fingerprints
2853	409	F06[N-Br]	frequency of N - Br at topological distance 06	2D frequency fingerprints
2854	410	F06[N-I]	frequency of N - I at topological distance 06	2D frequency fingerprints
2855	411	F06[N-B]	frequency of N - B at topological distance 06	2D frequency fingerprints
2856	412	F06[N-Si]	frequency of N - Si at topological distance 06	2D frequency fingerprints
2857	413	F06[N-X]	frequency of N - X at topological distance 06	2D frequency fingerprints
2858	414	F06[O-O]	frequency of O - O at topological distance 06	2D frequency fingerprints
2859	415	F06[O-S]	frequency of O - S at topological distance 06	2D frequency fingerprints
2860	416	F06[O-P]	frequency of O - P at topological distance 06	2D frequency fingerprints
2861	417	F06[O-F]	frequency of O - F at topological distance 06	2D frequency fingerprints

2862	418	F06[O-Cl]	frequency of O - Cl at topological distance 06	2D frequency fingerprints
2863	419	F06[O-Br]	frequency of O - Br at topological distance 06	2D frequency fingerprints
2864	420	F06[O-I]	frequency of O - I at topological distance 06	2D frequency fingerprints
2865	421	F06[O-B]	frequency of O - B at topological distance 06	2D frequency fingerprints
2866	422	F06[O-Si]	frequency of O - Si at topological distance 06	2D frequency fingerprints
2867	423	F06[O-X]	frequency of O - X at topological distance 06	2D frequency fingerprints
2868	424	F06[S-S]	frequency of S - S at topological distance 06	2D frequency fingerprints
2869	425	F06[S-P]	frequency of S - P at topological distance 06	2D frequency fingerprints
2870	426	F06[S-F]	frequency of S - F at topological distance 06	2D frequency fingerprints
2871	427	F06[S-Cl]	frequency of S - Cl at topological distance 06	2D frequency fingerprints
2872	428	F06[S-Br]	frequency of S - Br at topological distance 06	2D frequency fingerprints
2873	429	F06[S-I]	frequency of S - I at topological distance 06	2D frequency fingerprints
2874	430	F06[S-B]	frequency of S - B at topological distance 06	2D frequency fingerprints
2875	431	F06[S-Si]	frequency of S - Si at topological distance 06	2D frequency fingerprints
2876	432	F06[S-X]	frequency of S - X at topological distance 06	2D frequency fingerprints
2877	433	F06[P-P]	frequency of P - P at topological distance 06	2D frequency fingerprints
2878	434	F06[P-F]	frequency of P - F at topological distance 06	2D frequency fingerprints
2879	435	F06[P-Cl]	frequency of P - Cl at topological distance 06	2D frequency fingerprints

2880	436	F06[P-Br]	frequency of P - Br at topological distance 06	2D frequency fingerprints
2881	437	F06[P-I]	frequency of P - I at topological distance 06	2D frequency fingerprints
2882	438	F06[P-B]	frequency of P - B at topological distance 06	2D frequency fingerprints
2883	439	F06[P-Si]	frequency of P - Si at topological distance 06	2D frequency fingerprints
2884	440	F06[P-X]	frequency of P - X at topological distance 06	2D frequency fingerprints
2885	441	F06[F-F]	frequency of F - F at topological distance 06	2D frequency fingerprints
2886	442	F06[F-Cl]	frequency of F - Cl at topological distance 06	2D frequency fingerprints
2887	443	F06[F-Br]	frequency of F - Br at topological distance 06	2D frequency fingerprints
2888	444	F06[F-I]	frequency of F - I at topological distance 06	2D frequency fingerprints
2889	445	F06[F-B]	frequency of F - B at topological distance 06	2D frequency fingerprints
2890	446	F06[F-Si]	frequency of F - Si at topological distance 06	2D frequency fingerprints
2891	447	F06[F-X]	frequency of F - X at topological distance 06	2D frequency fingerprints
2892	448	F06[Cl-Cl]	frequency of Cl - Cl at topological distance 06	2D frequency fingerprints
2893	449	F06[Cl-Br]	frequency of Cl - Br at topological distance 06	2D frequency fingerprints
2894	450	F06[Cl-I]	frequency of Cl - I at topological distance 06	2D frequency fingerprints
2895	451	F06[Cl-B]	frequency of Cl - B at topological distance 06	2D frequency fingerprints
2896	452	F06[Cl-Si]	frequency of Cl - Si at topological distance 06	2D frequency fingerprints
2897	453	F06[Cl-X]	frequency of Cl - X at topological distance 06	2D frequency fingerprints

2898	454	F06[Br-Br]	frequency of Br - Br at topological distance 06	2D frequency fingerprints
2899	455	F06[Br-I]	frequency of Br - I at topological distance 06	2D frequency fingerprints
2900	456	F06[Br-B]	frequency of Br - B at topological distance 06	2D frequency fingerprints
2901	457	F06[Br-Si]	frequency of Br - Si at topological distance 06	2D frequency fingerprints
2902	458	F06[Br-X]	frequency of Br - X at topological distance 06	2D frequency fingerprints
2903	459	F06[I-I]	frequency of I - I at topological distance 06	2D frequency fingerprints
2904	460	F06[I-B]	frequency of I - B at topological distance 06	2D frequency fingerprints
2905	461	F06[I-Si]	frequency of I - Si at topological distance 06	2D frequency fingerprints
2906	462	F06[I-X]	frequency of I - X at topological distance 06	2D frequency fingerprints
2907	463	F06[B-B]	frequency of B - B at topological distance 06	2D frequency fingerprints
2908	464	F06[B-Si]	frequency of B - Si at topological distance 06	2D frequency fingerprints
2909	465	F06[B-X]	frequency of B - X at topological distance 06	2D frequency fingerprints
2910	466	F06[Si-Si]	frequency of Si - Si at topological distance 06	2D frequency fingerprints
2911	467	F06[Si-X]	frequency of Si - X at topological distance 06	2D frequency fingerprints
2912	468	F06[X-X]	frequency of X - X at topological distance 06	2D frequency fingerprints
2913	469	F07[C-C]	frequency of C - C at topological distance 07	2D frequency fingerprints
2914	470	F07[C-N]	frequency of C - N at topological distance 07	2D frequency fingerprints
2915	471	F07[C-O]	frequency of C - O at topological distance 07	2D frequency fingerprints

2916	472	F07[C-S]	frequency of C - S at topological distance 07	2D frequency fingerprints
2917	473	F07[C-P]	frequency of C - P at topological distance 07	2D frequency fingerprints
2918	474	F07[C-F]	frequency of C - F at topological distance 07	2D frequency fingerprints
2919	475	F07[C-Cl]	frequency of C - Cl at topological distance 07	2D frequency fingerprints
2920	476	F07[C-Br]	frequency of C - Br at topological distance 07	2D frequency fingerprints
2921	477	F07[C-I]	frequency of C - I at topological distance 07	2D frequency fingerprints
2922	478	F07[C-B]	frequency of C - B at topological distance 07	2D frequency fingerprints
2923	479	F07[C-Si]	frequency of C - Si at topological distance 07	2D frequency fingerprints
2924	480	F07[C-X]	frequency of C - X at topological distance 07	2D frequency fingerprints
2925	481	F07[N-N]	frequency of N - N at topological distance 07	2D frequency fingerprints
2926	482	F07[N-O]	frequency of N - O at topological distance 07	2D frequency fingerprints
2927	483	F07[N-S]	frequency of N - S at topological distance 07	2D frequency fingerprints
2928	484	F07[N-P]	frequency of N - P at topological distance 07	2D frequency fingerprints
2929	485	F07[N-F]	frequency of N - F at topological distance 07	2D frequency fingerprints
2930	486	F07[N-Cl]	frequency of N - Cl at topological distance 07	2D frequency fingerprints
2931	487	F07[N-Br]	frequency of N - Br at topological distance 07	2D frequency fingerprints
2932	488	F07[N-I]	frequency of N - I at topological distance 07	2D frequency fingerprints
2933	489	F07[N-B]	frequency of N - B at topological distance 07	2D frequency fingerprints

2934	490	F07[N-Si]	frequency of N - Si at topological distance 07	2D frequency fingerprints
2935	491	F07[N-X]	frequency of N - X at topological distance 07	2D frequency fingerprints
2936	492	F07[O-O]	frequency of O - O at topological distance 07	2D frequency fingerprints
2937	493	F07[O-S]	frequency of O - S at topological distance 07	2D frequency fingerprints
2938	494	F07[O-P]	frequency of O - P at topological distance 07	2D frequency fingerprints
2939	495	F07[O-F]	frequency of O - F at topological distance 07	2D frequency fingerprints
2940	496	F07[O-Cl]	frequency of O - Cl at topological distance 07	2D frequency fingerprints
2941	497	F07[O-Br]	frequency of O - Br at topological distance 07	2D frequency fingerprints
2942	498	F07[O-I]	frequency of O - I at topological distance 07	2D frequency fingerprints
2943	499	F07[O-B]	frequency of O - B at topological distance 07	2D frequency fingerprints
2944	500	F07[O-Si]	frequency of O - Si at topological distance 07	2D frequency fingerprints
2945	501	F07[O-X]	frequency of O - X at topological distance 07	2D frequency fingerprints
2946	502	F07[S-S]	frequency of S - S at topological distance 07	2D frequency fingerprints
2947	503	F07[S-P]	frequency of S - P at topological distance 07	2D frequency fingerprints
2948	504	F07[S-F]	frequency of S - F at topological distance 07	2D frequency fingerprints
2949	505	F07[S-Cl]	frequency of S - Cl at topological distance 07	2D frequency fingerprints
2950	506	F07[S-Br]	frequency of S - Br at topological distance 07	2D frequency fingerprints
2951	507	F07[S-I]	frequency of S - I at topological distance 07	2D frequency fingerprints

2952	508	F07[S-B]	frequency of S - B at topological distance 07	2D frequency fingerprints
2953	509	F07[S-Si]	frequency of S - Si at topological distance 07	2D frequency fingerprints
2954	510	F07[S-X]	frequency of S - X at topological distance 07	2D frequency fingerprints
2955	511	F07[P-P]	frequency of P - P at topological distance 07	2D frequency fingerprints
2956	512	F07[P-F]	frequency of P - F at topological distance 07	2D frequency fingerprints
2957	513	F07[P-Cl]	frequency of P - Cl at topological distance 07	2D frequency fingerprints
2958	514	F07[P-Br]	frequency of P - Br at topological distance 07	2D frequency fingerprints
2959	515	F07[P-I]	frequency of P - I at topological distance 07	2D frequency fingerprints
2960	516	F07[P-B]	frequency of P - B at topological distance 07	2D frequency fingerprints
2961	517	F07[P-Si]	frequency of P - Si at topological distance 07	2D frequency fingerprints
2962	518	F07[P-X]	frequency of P - X at topological distance 07	2D frequency fingerprints
2963	519	F07[F-F]	frequency of F - F at topological distance 07	2D frequency fingerprints
2964	520	F07[F-Cl]	frequency of F - Cl at topological distance 07	2D frequency fingerprints
2965	521	F07[F-Br]	frequency of F - Br at topological distance 07	2D frequency fingerprints
2966	522	F07[F-I]	frequency of F - I at topological distance 07	2D frequency fingerprints
2967	523	F07[F-B]	frequency of F - B at topological distance 07	2D frequency fingerprints
2968	524	F07[F-Si]	frequency of F - Si at topological distance 07	2D frequency fingerprints
2969	525	F07[F-X]	frequency of F - X at topological distance 07	2D frequency fingerprints

2970	526	F07[Cl-Cl]	frequency of Cl - Cl at topological distance 07	2D frequency fingerprints
2971	527	F07[Cl-Br]	frequency of Cl - Br at topological distance 07	2D frequency fingerprints
2972	528	F07[Cl-I]	frequency of Cl - I at topological distance 07	2D frequency fingerprints
2973	529	F07[Cl-B]	frequency of Cl - B at topological distance 07	2D frequency fingerprints
2974	530	F07[Cl-Si]	frequency of Cl - Si at topological distance 07	2D frequency fingerprints
2975	531	F07[Cl-X]	frequency of Cl - X at topological distance 07	2D frequency fingerprints
2976	532	F07[Br-Br]	frequency of Br - Br at topological distance 07	2D frequency fingerprints
2977	533	F07[Br-I]	frequency of Br - I at topological distance 07	2D frequency fingerprints
2978	534	F07[Br-B]	frequency of Br - B at topological distance 07	2D frequency fingerprints
2979	535	F07[Br-Si]	frequency of Br - Si at topological distance 07	2D frequency fingerprints
2980	536	F07[Br-X]	frequency of Br - X at topological distance 07	2D frequency fingerprints
2981	537	F07[I-I]	frequency of I - I at topological distance 07	2D frequency fingerprints
2982	538	F07[I-B]	frequency of I - B at topological distance 07	2D frequency fingerprints
2983	539	F07[I-Si]	frequency of I - Si at topological distance 07	2D frequency fingerprints
2984	540	F07[I-X]	frequency of I - X at topological distance 07	2D frequency fingerprints
2985	541	F07[B-B]	frequency of B - B at topological distance 07	2D frequency fingerprints
2986	542	F07[B-Si]	frequency of B - Si at topological distance 07	2D frequency fingerprints
2987	543	F07[B-X]	frequency of B - X at topological distance 07	2D frequency fingerprints

2988	544	F07[Si-Si]	frequency of Si - Si at topological distance 07	2D frequency fingerprints
2989	545	F07[Si-X]	frequency of Si - X at topological distance 07	2D frequency fingerprints
2990	546	F07[X-X]	frequency of X - X at topological distance 07	2D frequency fingerprints
2991	547	F08[C-C]	frequency of C - C at topological distance 08	2D frequency fingerprints
2992	548	F08[C-N]	frequency of C - N at topological distance 08	2D frequency fingerprints
2993	549	F08[C-O]	frequency of C - O at topological distance 08	2D frequency fingerprints
2994	550	F08[C-S]	frequency of C - S at topological distance 08	2D frequency fingerprints
2995	551	F08[C-P]	frequency of C - P at topological distance 08	2D frequency fingerprints
2996	552	F08[C-F]	frequency of C - F at topological distance 08	2D frequency fingerprints
2997	553	F08[C-Cl]	frequency of C - Cl at topological distance 08	2D frequency fingerprints
2998	554	F08[C-Br]	frequency of C - Br at topological distance 08	2D frequency fingerprints
2999	555	F08[C-I]	frequency of C - I at topological distance 08	2D frequency fingerprints
3000	556	F08[C-B]	frequency of C - B at topological distance 08	2D frequency fingerprints
3001	557	F08[C-Si]	frequency of C - Si at topological distance 08	2D frequency fingerprints
3002	558	F08[C-X]	frequency of C - X at topological distance 08	2D frequency fingerprints
3003	559	F08[N-N]	frequency of N - N at topological distance 08	2D frequency fingerprints
3004	560	F08[N-O]	frequency of N - O at topological distance 08	2D frequency fingerprints
3005	561	F08[N-S]	frequency of N - S at topological distance 08	2D frequency fingerprints

3006	562	F08[N-P]	frequency of N - P at topological distance 08	2D frequency fingerprints
3007	563	F08[N-F]	frequency of N - F at topological distance 08	2D frequency fingerprints
3008	564	F08[N-Cl]	frequency of N - Cl at topological distance 08	2D frequency fingerprints
3009	565	F08[N-Br]	frequency of N - Br at topological distance 08	2D frequency fingerprints
3010	566	F08[N-I]	frequency of N - I at topological distance 08	2D frequency fingerprints
3011	567	F08[N-B]	frequency of N - B at topological distance 08	2D frequency fingerprints
3012	568	F08[N-Si]	frequency of N - Si at topological distance 08	2D frequency fingerprints
3013	569	F08[N-X]	frequency of N - X at topological distance 08	2D frequency fingerprints
3014	570	F08[O-O]	frequency of O - O at topological distance 08	2D frequency fingerprints
3015	571	F08[O-S]	frequency of O - S at topological distance 08	2D frequency fingerprints
3016	572	F08[O-P]	frequency of O - P at topological distance 08	2D frequency fingerprints
3017	573	F08[O-F]	frequency of O - F at topological distance 08	2D frequency fingerprints
3018	574	F08[O-Cl]	frequency of O - Cl at topological distance 08	2D frequency fingerprints
3019	575	F08[O-Br]	frequency of O - Br at topological distance 08	2D frequency fingerprints
3020	576	F08[O-I]	frequency of O - I at topological distance 08	2D frequency fingerprints
3021	577	F08[O-B]	frequency of O - B at topological distance 08	2D frequency fingerprints
3022	578	F08[O-Si]	frequency of O - Si at topological distance 08	2D frequency fingerprints
3023	579	F08[O-X]	frequency of O - X at topological distance 08	2D frequency fingerprints

3024	580	F08[S-S]	frequency of S - S at topological distance 08	2D frequency fingerprints
3025	581	F08[S-P]	frequency of S - P at topological distance 08	2D frequency fingerprints
3026	582	F08[S-F]	frequency of S - F at topological distance 08	2D frequency fingerprints
3027	583	F08[S-Cl]	frequency of S - Cl at topological distance 08	2D frequency fingerprints
3028	584	F08[S-Br]	frequency of S - Br at topological distance 08	2D frequency fingerprints
3029	585	F08[S-I]	frequency of S - I at topological distance 08	2D frequency fingerprints
3030	586	F08[S-B]	frequency of S - B at topological distance 08	2D frequency fingerprints
3031	587	F08[S-Si]	frequency of S - Si at topological distance 08	2D frequency fingerprints
3032	588	F08[S-X]	frequency of S - X at topological distance 08	2D frequency fingerprints
3033	589	F08[P-P]	frequency of P - P at topological distance 08	2D frequency fingerprints
3034	590	F08[P-F]	frequency of P - F at topological distance 08	2D frequency fingerprints
3035	591	F08[P-Cl]	frequency of P - Cl at topological distance 08	2D frequency fingerprints
3036	592	F08[P-Br]	frequency of P - Br at topological distance 08	2D frequency fingerprints
3037	593	F08[P-I]	frequency of P - I at topological distance 08	2D frequency fingerprints
3038	594	F08[P-B]	frequency of P - B at topological distance 08	2D frequency fingerprints
3039	595	F08[P-Si]	frequency of P - Si at topological distance 08	2D frequency fingerprints
3040	596	F08[P-X]	frequency of P - X at topological distance 08	2D frequency fingerprints
3041	597	F08[F-F]	frequency of F - F at topological distance 08	2D frequency fingerprints

3042	598	F08[F-Cl]	frequency of F - Cl at topological distance 08	2D frequency fingerprints
3043	599	F08[F-Br]	frequency of F - Br at topological distance 08	2D frequency fingerprints
3044	600	F08[F-I]	frequency of F - I at topological distance 08	2D frequency fingerprints
3045	601	F08[F-B]	frequency of F - B at topological distance 08	2D frequency fingerprints
3046	602	F08[F-Si]	frequency of F - Si at topological distance 08	2D frequency fingerprints
3047	603	F08[F-X]	frequency of F - X at topological distance 08	2D frequency fingerprints
3048	604	F08[Cl-Cl]	frequency of Cl - Cl at topological distance 08	2D frequency fingerprints
3049	605	F08[Cl-Br]	frequency of Cl - Br at topological distance 08	2D frequency fingerprints
3050	606	F08[Cl-I]	frequency of Cl - I at topological distance 08	2D frequency fingerprints
3051	607	F08[Cl-B]	frequency of Cl - B at topological distance 08	2D frequency fingerprints
3052	608	F08[Cl-Si]	frequency of Cl - Si at topological distance 08	2D frequency fingerprints
3053	609	F08[Cl-X]	frequency of Cl - X at topological distance 08	2D frequency fingerprints
3054	610	F08[Br-Br]	frequency of Br - Br at topological distance 08	2D frequency fingerprints
3055	611	F08[Br-I]	frequency of Br - I at topological distance 08	2D frequency fingerprints
3056	612	F08[Br-B]	frequency of Br - B at topological distance 08	2D frequency fingerprints
3057	613	F08[Br-Si]	frequency of Br - Si at topological distance 08	2D frequency fingerprints
3058	614	F08[Br-X]	frequency of Br - X at topological distance 08	2D frequency fingerprints
3059	615	F08[I-I]	frequency of I - I at topological distance 08	2D frequency fingerprints

3060	616	F08[I-B]	frequency of I - B at topological distance 08	2D frequency fingerprints
3061	617	F08[I-Si]	frequency of I - Si at topological distance 08	2D frequency fingerprints
3062	618	F08[I-X]	frequency of I - X at topological distance 08	2D frequency fingerprints
3063	619	F08[B-B]	frequency of B - B at topological distance 08	2D frequency fingerprints
3064	620	F08[B-Si]	frequency of B - Si at topological distance 08	2D frequency fingerprints
3065	621	F08[B-X]	frequency of B - X at topological distance 08	2D frequency fingerprints
3066	622	F08[Si-Si]	frequency of Si - Si at topological distance 08	2D frequency fingerprints
3067	623	F08[Si-X]	frequency of Si - X at topological distance 08	2D frequency fingerprints
3068	624	F08[X-X]	frequency of X - X at topological distance 08	2D frequency fingerprints
3069	625	F09[C-C]	frequency of C - C at topological distance 09	2D frequency fingerprints
3070	626	F09[C-N]	frequency of C - N at topological distance 09	2D frequency fingerprints
3071	627	F09[C-O]	frequency of C - O at topological distance 09	2D frequency fingerprints
3072	628	F09[C-S]	frequency of C - S at topological distance 09	2D frequency fingerprints
3073	629	F09[C-P]	frequency of C - P at topological distance 09	2D frequency fingerprints
3074	630	F09[C-F]	frequency of C - F at topological distance 09	2D frequency fingerprints
3075	631	F09[C-Cl]	frequency of C - Cl at topological distance 09	2D frequency fingerprints
3076	632	F09[C-Br]	frequency of C - Br at topological distance 09	2D frequency fingerprints
3077	633	F09[C-I]	frequency of C - I at topological distance 09	2D frequency fingerprints

3078	634	F09[C-B]	frequency of C - B at topological distance 09	2D frequency fingerprints
3079	635	F09[C-Si]	frequency of C - Si at topological distance 09	2D frequency fingerprints
3080	636	F09[C-X]	frequency of C - X at topological distance 09	2D frequency fingerprints
3081	637	F09[N-N]	frequency of N - N at topological distance 09	2D frequency fingerprints
3082	638	F09[N-O]	frequency of N - O at topological distance 09	2D frequency fingerprints
3083	639	F09[N-S]	frequency of N - S at topological distance 09	2D frequency fingerprints
3084	640	F09[N-P]	frequency of N - P at topological distance 09	2D frequency fingerprints
3085	641	F09[N-F]	frequency of N - F at topological distance 09	2D frequency fingerprints
3086	642	F09[N-Cl]	frequency of N - Cl at topological distance 09	2D frequency fingerprints
3087	643	F09[N-Br]	frequency of N - Br at topological distance 09	2D frequency fingerprints
3088	644	F09[N-I]	frequency of N - I at topological distance 09	2D frequency fingerprints
3089	645	F09[N-B]	frequency of N - B at topological distance 09	2D frequency fingerprints
3090	646	F09[N-Si]	frequency of N - Si at topological distance 09	2D frequency fingerprints
3091	647	F09[N-X]	frequency of N - X at topological distance 09	2D frequency fingerprints
3092	648	F09[O-O]	frequency of O - O at topological distance 09	2D frequency fingerprints
3093	649	F09[O-S]	frequency of O - S at topological distance 09	2D frequency fingerprints
3094	650	F09[O-P]	frequency of O - P at topological distance 09	2D frequency fingerprints
3095	651	F09[O-F]	frequency of O - F at topological distance 09	2D frequency fingerprints

3096	652	F09[O-Cl]	frequency of O - Cl at topological distance 09	2D frequency fingerprints
3097	653	F09[O-Br]	frequency of O - Br at topological distance 09	2D frequency fingerprints
3098	654	F09[O-I]	frequency of O - I at topological distance 09	2D frequency fingerprints
3099	655	F09[O-B]	frequency of O - B at topological distance 09	2D frequency fingerprints
3100	656	F09[O-Si]	frequency of O - Si at topological distance 09	2D frequency fingerprints
3101	657	F09[O-X]	frequency of O - X at topological distance 09	2D frequency fingerprints
3102	658	F09[S-S]	frequency of S - S at topological distance 09	2D frequency fingerprints
3103	659	F09[S-P]	frequency of S - P at topological distance 09	2D frequency fingerprints
3104	660	F09[S-F]	frequency of S - F at topological distance 09	2D frequency fingerprints
3105	661	F09[S-Cl]	frequency of S - Cl at topological distance 09	2D frequency fingerprints
3106	662	F09[S-Br]	frequency of S - Br at topological distance 09	2D frequency fingerprints
3107	663	F09[S-I]	frequency of S - I at topological distance 09	2D frequency fingerprints
3108	664	F09[S-B]	frequency of S - B at topological distance 09	2D frequency fingerprints
3109	665	F09[S-Si]	frequency of S - Si at topological distance 09	2D frequency fingerprints
3110	666	F09[S-X]	frequency of S - X at topological distance 09	2D frequency fingerprints
3111	667	F09[P-P]	frequency of P - P at topological distance 09	2D frequency fingerprints
3112	668	F09[P-F]	frequency of P - F at topological distance 09	2D frequency fingerprints
3113	669	F09[P-Cl]	frequency of P - Cl at topological distance 09	2D frequency fingerprints

3114	670	F09[P-Br]	frequency of P - Br at topological distance 09	2D frequency fingerprints
3115	671	F09[P-I]	frequency of P - I at topological distance 09	2D frequency fingerprints
3116	672	F09[P-B]	frequency of P - B at topological distance 09	2D frequency fingerprints
3117	673	F09[P-Si]	frequency of P - Si at topological distance 09	2D frequency fingerprints
3118	674	F09[P-X]	frequency of P - X at topological distance 09	2D frequency fingerprints
3119	675	F09[F-F]	frequency of F - F at topological distance 09	2D frequency fingerprints
3120	676	F09[F-Cl]	frequency of F - Cl at topological distance 09	2D frequency fingerprints
3121	677	F09[F-Br]	frequency of F - Br at topological distance 09	2D frequency fingerprints
3122	678	F09[F-I]	frequency of F - I at topological distance 09	2D frequency fingerprints
3123	679	F09[F-B]	frequency of F - B at topological distance 09	2D frequency fingerprints
3124	680	F09[F-Si]	frequency of F - Si at topological distance 09	2D frequency fingerprints
3125	681	F09[F-X]	frequency of F - X at topological distance 09	2D frequency fingerprints
3126	682	F09[Cl-Cl]	frequency of Cl - Cl at topological distance 09	2D frequency fingerprints
3127	683	F09[Cl-Br]	frequency of Cl - Br at topological distance 09	2D frequency fingerprints
3128	684	F09[Cl-I]	frequency of Cl - I at topological distance 09	2D frequency fingerprints
3129	685	F09[Cl-B]	frequency of Cl - B at topological distance 09	2D frequency fingerprints
3130	686	F09[Cl-Si]	frequency of Cl - Si at topological distance 09	2D frequency fingerprints
3131	687	F09[Cl-X]	frequency of Cl - X at topological distance 09	2D frequency fingerprints

3132	688	F09[Br-Br]	frequency of Br - Br at topological distance 09	2D frequency fingerprints
3133	689	F09[Br-I]	frequency of Br - I at topological distance 09	2D frequency fingerprints
3134	690	F09[Br-B]	frequency of Br - B at topological distance 09	2D frequency fingerprints
3135	691	F09[Br-Si]	frequency of Br - Si at topological distance 09	2D frequency fingerprints
3136	692	F09[Br-X]	frequency of Br - X at topological distance 09	2D frequency fingerprints
3137	693	F09[I-I]	frequency of I - I at topological distance 09	2D frequency fingerprints
3138	694	F09[I-B]	frequency of I - B at topological distance 09	2D frequency fingerprints
3139	695	F09[I-Si]	frequency of I - Si at topological distance 09	2D frequency fingerprints
3140	696	F09[I-X]	frequency of I - X at topological distance 09	2D frequency fingerprints
3141	697	F09[B-B]	frequency of B - B at topological distance 09	2D frequency fingerprints
3142	698	F09[B-Si]	frequency of B - Si at topological distance 09	2D frequency fingerprints
3143	699	F09[B-X]	frequency of B - X at topological distance 09	2D frequency fingerprints
3144	700	F09[Si-Si]	frequency of Si - Si at topological distance 09	2D frequency fingerprints
3145	701	F09[Si-X]	frequency of Si - X at topological distance 09	2D frequency fingerprints
3146	702	F09[X-X]	frequency of X - X at topological distance 09	2D frequency fingerprints
3147	703	F10[C-C]	frequency of C - C at topological distance 10	2D frequency fingerprints
3148	704	F10[C-N]	frequency of C - N at topological distance 10	2D frequency fingerprints
3149	705	F10[C-O]	frequency of C - O at topological distance 10	2D frequency fingerprints

3150	706	F10[C-S]	frequency of C - S at topological distance 10	2D frequency fingerprints
3151	707	F10[C-P]	frequency of C - P at topological distance 10	2D frequency fingerprints
3152	708	F10[C-F]	frequency of C - F at topological distance 10	2D frequency fingerprints
3153	709	F10[C-Cl]	frequency of C - Cl at topological distance 10	2D frequency fingerprints
3154	710	F10[C-Br]	frequency of C - Br at topological distance 10	2D frequency fingerprints
3155	711	F10[C-I]	frequency of C - I at topological distance 10	2D frequency fingerprints
3156	712	F10[C-B]	frequency of C - B at topological distance 10	2D frequency fingerprints
3157	713	F10[C-Si]	frequency of C - Si at topological distance 10	2D frequency fingerprints
3158	714	F10[C-X]	frequency of C - X at topological distance 10	2D frequency fingerprints
3159	715	F10[N-N]	frequency of N - N at topological distance 10	2D frequency fingerprints
3160	716	F10[N-O]	frequency of N - O at topological distance 10	2D frequency fingerprints
3161	717	F10[N-S]	frequency of N - S at topological distance 10	2D frequency fingerprints
3162	718	F10[N-P]	frequency of N - P at topological distance 10	2D frequency fingerprints
3163	719	F10[N-F]	frequency of N - F at topological distance 10	2D frequency fingerprints
3164	720	F10[N-Cl]	frequency of N - Cl at topological distance 10	2D frequency fingerprints
3165	721	F10[N-Br]	frequency of N - Br at topological distance 10	2D frequency fingerprints
3166	722	F10[N-I]	frequency of N - I at topological distance 10	2D frequency fingerprints
3167	723	F10[N-B]	frequency of N - B at topological distance 10	2D frequency fingerprints

3168	724	F10[N-Si]	frequency of N - Si at topological distance 10	2D frequency fingerprints
3169	725	F10[N-X]	frequency of N - X at topological distance 10	2D frequency fingerprints
3170	726	F10[O-O]	frequency of O - O at topological distance 10	2D frequency fingerprints
3171	727	F10[O-S]	frequency of O - S at topological distance 10	2D frequency fingerprints
3172	728	F10[O-P]	frequency of O - P at topological distance 10	2D frequency fingerprints
3173	729	F10[O-F]	frequency of O - F at topological distance 10	2D frequency fingerprints
3174	730	F10[O-Cl]	frequency of O - Cl at topological distance 10	2D frequency fingerprints
3175	731	F10[O-Br]	frequency of O - Br at topological distance 10	2D frequency fingerprints
3176	732	F10[O-I]	frequency of O - I at topological distance 10	2D frequency fingerprints
3177	733	F10[O-B]	frequency of O - B at topological distance 10	2D frequency fingerprints
3178	734	F10[O-Si]	frequency of O - Si at topological distance 10	2D frequency fingerprints
3179	735	F10[O-X]	frequency of O - X at topological distance 10	2D frequency fingerprints
3180	736	F10[S-S]	frequency of S - S at topological distance 10	2D frequency fingerprints
3181	737	F10[S-P]	frequency of S - P at topological distance 10	2D frequency fingerprints
3182	738	F10[S-F]	frequency of S - F at topological distance 10	2D frequency fingerprints
3183	739	F10[S-Cl]	frequency of S - Cl at topological distance 10	2D frequency fingerprints
3184	740	F10[S-Br]	frequency of S - Br at topological distance 10	2D frequency fingerprints
3185	741	F10[S-I]	frequency of S - I at topological distance 10	2D frequency fingerprints

3186	742	F10[S-B]	frequency of S - B at topological distance 10	2D frequency fingerprints
3187	743	F10[S-Si]	frequency of S - Si at topological distance 10	2D frequency fingerprints
3188	744	F10[S-X]	frequency of S - X at topological distance 10	2D frequency fingerprints
3189	745	F10[P-P]	frequency of P - P at topological distance 10	2D frequency fingerprints
3190	746	F10[P-F]	frequency of P - F at topological distance 10	2D frequency fingerprints
3191	747	F10[P-Cl]	frequency of P - Cl at topological distance 10	2D frequency fingerprints
3192	748	F10[P-Br]	frequency of P - Br at topological distance 10	2D frequency fingerprints
3193	749	F10[P-I]	frequency of P - I at topological distance 10	2D frequency fingerprints
3194	750	F10[P-B]	frequency of P - B at topological distance 10	2D frequency fingerprints
3195	751	F10[P-Si]	frequency of P - Si at topological distance 10	2D frequency fingerprints
3196	752	F10[P-X]	frequency of P - X at topological distance 10	2D frequency fingerprints
3197	753	F10[F-F]	frequency of F - F at topological distance 10	2D frequency fingerprints
3198	754	F10[F-Cl]	frequency of F - Cl at topological distance 10	2D frequency fingerprints
3199	755	F10[F-Br]	frequency of F - Br at topological distance 10	2D frequency fingerprints
3200	756	F10[F-I]	frequency of F - I at topological distance 10	2D frequency fingerprints
3201	757	F10[F-B]	frequency of F - B at topological distance 10	2D frequency fingerprints
3202	758	F10[F-Si]	frequency of F - Si at topological distance 10	2D frequency fingerprints
3203	759	F10[F-X]	frequency of F - X at topological distance 10	2D frequency fingerprints

3204	760	F10[Cl-Cl]	frequency of Cl - Cl at topological distance 10	2D frequency fingerprints
3205	761	F10[Cl-Br]	frequency of Cl - Br at topological distance 10	2D frequency fingerprints
3206	762	F10[Cl-I]	frequency of Cl - I at topological distance 10	2D frequency fingerprints
3207	763	F10[Cl-B]	frequency of Cl - B at topological distance 10	2D frequency fingerprints
3208	764	F10[Cl-Si]	frequency of Cl - Si at topological distance 10	2D frequency fingerprints
3209	765	F10[Cl-X]	frequency of Cl - X at topological distance 10	2D frequency fingerprints
3210	766	F10[Br-Br]	frequency of Br - Br at topological distance 10	2D frequency fingerprints
3211	767	F10[Br-I]	frequency of Br - I at topological distance 10	2D frequency fingerprints
3212	768	F10[Br-B]	frequency of Br - B at topological distance 10	2D frequency fingerprints
3213	769	F10[Br-Si]	frequency of Br - Si at topological distance 10	2D frequency fingerprints
3214	770	F10[Br-X]	frequency of Br - X at topological distance 10	2D frequency fingerprints
3215	771	F10[I-I]	frequency of I - I at topological distance 10	2D frequency fingerprints
3216	772	F10[I-B]	frequency of I - B at topological distance 10	2D frequency fingerprints
3217	773	F10[I-Si]	frequency of I - Si at topological distance 10	2D frequency fingerprints
3218	774	F10[I-X]	frequency of I - X at topological distance 10	2D frequency fingerprints
3219	775	F10[B-B]	frequency of B - B at topological distance 10	2D frequency fingerprints
3220	776	F10[B-Si]	frequency of B - Si at topological distance 10	2D frequency fingerprints
3221	777	F10[B-X]	frequency of B - X at topological distance 10	2D frequency fingerprints

3222	778	F10[Si-Si]	frequency of Si - Si at topological distance 10	2D frequency fingerprints
3223	779	F10[Si-X]	frequency of Si - X at topological distance 10	2D frequency fingerprints
3224	780	F10[X-X]	frequency of X - X at topological distance 10	2D frequency fingerprints