

List of molecular descriptors calculated by Dragon

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



93 BBI Bertz branching index Topological indices 94 DBI Dragon branching index Topological indices 95 96 SNa Narumi simple topological index (log function) Topological indices HNar Narumi harmonic topological index Topological indices 97 Narumi geometric topological index Topological indices GNa 98 Xt total structure connectivity index Topological indices 99 Topological indices Dz Pogliani index ramification index
Kier benzene-likeliness index Topological indices
Topological indices 100 Ram 101 BLI polarity number log of product of row sums (PRS) 102 Topological indices LPRS 103 Topological indices mean square distance index (Balaban) 104 MSD Topological indices superpendentic index 2D Petitjean shape index Topological indices Topological indices 105 SPI 106 PJI2 107 108 ECC eccentricity Topological indices AECC average eccentricity Topological indices 109 DECC Topological indices 110 111 Topological indices Topological indices MDDD mean distance degree deviation UNIF unipolarity Topological indices
Topological indices 112 CENT centralization 113 VAR variation 114 ICR radial centric information index Topological indices Topological indices Topological indices 115 SMTI Schultz Molecular Topological Index (MTI) Schultz Molecular Topological Index by valence vertex degrees 116 SMTIV 117 **GMTI** Gutman Molecular Topological Index Topological indices 118 GMTIV Gutman Molecular Topological Index by valence vertex degrees Topological indices 119 120 Xu CSI Topological indices eccentric connectivity index Topological indices 121 all-path Wiener index Wap Topological indices 1-path Kier alpha-modified shape index Topological indices
Topological indices S1K 123 S2K 2-path Kier alpha-modified shape index 124 125 S3K PHI 3-path Kier alpha-modified shape index Topological indices Kier flexibility index Topological indices 126 PW2 path/walk 2 - Randic shape index Topological indices path/walk 3 - Randic shape index path/walk 4 - Randic shape index 127 PW3 Topological indices 128 PW4 Topological indices Topological indices Topological indices 129 PW5 path/walk 5 - Randic shape index MAXDN maximal electrotopological negative variation 130 131 MAXDP maximal electrotopological positive variation Topological indices 132 DELS molecular electrotopological variation Topological indices 133 TIE E-state topological parameter Topological indices 134 135 intrinsic state pseudoconnectivity index - type S intrinsic state pseudoconnectivity index - type S average Topological indices
Topological indices Psi_i_s Psi i A 136 Psi_i_0 intrinsic state pseudoconnectivity index - type 0 Topological indices Psi_i_1 Psi_i_t 137 intrinsic state pseudoconnectivity index - type 1 Topological indices 138 intrinsic state pseudoconnectivity index - type T Topological indices Psi_i_0d Psi_i_1d Topological indices Topological indices 139 intrinsic state pseudoconnectivity index - type 0d 140 intrinsic state pseudoconnectivity index - type 1d 141 142 Psi_i_1s intrinsic state pseudoconnectivity index - type 1s electrotopological state pseudoconnectivity index - type S average Topological indices
Topological indices Psi_e_A 143 Psi_e_0 electrotopological state pseudoconnectivity index - type 0 Topological indices 144 Psi_e_1 Psi_e_t electrotopological state pseudoconnectivity index - type 1 Topological indices 145 electrotopological state pseudoconnectivity index - type T Topological indices 146 147 electrotopological state pseudoconnectivity index - type 0d electrotopological state pseudoconnectivity index - type 1d Topological indices Topological indices Psi_e_0d Psi_e_1d 148 149 Psi_e_1s electrotopological state pseudoconnectivity index - type 1s Topological indices BAC Balaban centric index Topological indices 150 LOC Topological indices lopping centric index 151 MWC01 molecular walk count of order 1 Walk and path counts Walk and path counts 152 MWC02 molecular walk count of order 2 153 MWC03 molecular walk count of order 3 Walk and path counts MWC04 molecular walk count of order 4 154 Walk and path counts 155 MWC05 molecular walk count of order 5 Walk and path counts 156 MWC06 molecular walk count of order 6 Walk and path counts 157 MWC07 molecular walk count of order 7 Walk and path counts 158 159 MWC08 MWC09 molecular walk count of order 8 Walk and path counts molecular walk count of order 9 Walk and path counts 160 MWC10 molecular walk count of order 10 Walk and path counts 161 SRW02 self-returning walk count of order 2 Walk and path counts SRW03 self-returning walk count of order 3 162 Walk and path counts 163 SRW04 self-returning walk count of order 4 self-returning walk count of order 5 Walk and path counts SRW05 164 Walk and path counts SRW06 SRW07 165 self-returning walk count of order 6 Walk and path counts self-returning walk count of order 7 166 Walk and path counts SRW08 self-returning walk count of order 8 167 Walk and path counts self-returning walk count of order 9 self-returning walk count of order 10 168 SRW09 Walk and path counts 169 SRW10 Walk and path counts MPC01 MPC02 molecular path count of order 1 (no. of non-H bonds) molecular path count of order 2 (Gordon-Scantlebury index) 170 Walk and path counts 171 Walk and path counts 172 MPC03 molecular path count of order 3 Walk and path counts MPC04 173 molecular path count of order 4 Walk and path counts MPC05 molecular path count of order 5 174 Walk and path counts 175 176 MPC06 MPC07 molecular path count of order 6 molecular path count of order 7 Walk and path counts Walk and path counts 177 MPC08 molecular path count of order 8 Walk and path counts 178 MPC09 molecular path count of order 9 molecular path count of order 10 Walk and path counts Walk and path counts 179 MPC10 piPC01 piPC02 molecular multiple path count of order 1 molecular multiple path count of order 2 180 Walk and path counts 181 Walk and path counts 182 183 piPC03 piPC04 molecular multiple path count of order 3 molecular multiple path count of order 4 Walk and path counts Walk and path counts piPC05 molecular multiple path count of order 5 184 Walk and path counts 185 niPC06 molecular multiple path count of order 6 Walk and path counts 186 piPC07 molecular multiple path count of order 7 Walk and path counts piPC08 187 molecular multiple path count of order 8 Walk and path counts piPC09 molecular multiple path count of order 9 188 Walk and path counts



piPC10 molecular multiple path count of order 10 Walk and path counts 189 TWC 190 total walk coun Walk and path counts 191 TPC total path count Walk and path counts 192 piID conventional bond order ID number Walk and path counts 193 194 PCR PCD ratio of multiple path count over path coun Walk and path counts difference between multiple path count and path count Walk and path counts 195 CID Randic ID number Walk and path counts 196 197 BID Balaban ID number Walk and path counts connectivity index of order 0 Connectivity indices X0 connectivity index of order 1 (Randic connectivity index) connectivity index of order 2 198 199 X1 X2 Connectivity indices Connectivity indices X3 X4 X5 200 connectivity index of order 3 Connectivity indices 201 202 connectivity index of order 4 connectivity index of order 5 Connectivity indices Connectivity indices 203 204 X0A average connectivity index of order 0 Connectivity indices average connectivity index of order 1 Connectivity indices X1A 205 X2A average connectivity index of order 2 Connectivity indices average connectivity index of order 3 average connectivity index of order 4 206 X3A Connectivity indices 207 X4A Connectivity indices 208 209 X5A average connectivity index of order 5 Connectivity indices valence connectivity index of order 0 X0v Connectivity indices 210 X1v valence connectivity index of order 1 Connectivity indices 211 212 valence connectivity index of order 2 valence connectivity index of order 3 X2v Connectivity indices Connectivity indices valence connectivity index of order 4 valence connectivity index of order 5 213 X4v Connectivity indices 214 Connectivity indices X5v 215 216 average valence connectivity index of order 0 average valence connectivity index of order 1 X0A_V Connectivity indices Connectivity indices X1Av 217 average valence connectivity index of order 2 Connectivity indices X2Av 218 X3Av average valence connectivity index of order 3 Connectivity indices 219 X4Av average valence connectivity index of order 4 Connectivity indices 220 221 X5Av average valence connectivity index of order 5 solvation connectivity index of order 0 Connectivity indices X0so Connectivity indices Connectivity indices 222 X1sol solvation connectivity index of order 1 223 224 X2sol solvation connectivity index of order 2 solvation connectivity index of order 3 Connectivity indices Connectivity indices X3sol solvation connectivity index of order 4 solvation connectivity index of order 5 225 X4sol Connectivity indices 226 Connectivity indices X5sol 227 228 XMOD modified Randic index Connectivity indices **RDCHI** reciprocal distance sum Randic-like index Connectivity indices 229 RDSQ reciprocal distance sum inverse Randic-like index Connectivity indices 230 231 X1Kup X1Mad Kupchik connectivity index connectivity topochemical index Connectivity indices Connectivity indices 232 X1Per perturbation connectivity index Connectivity indices 233 X1MulPer multiplicative perturbation connectivity index Connectivity indices 234 ISIZ information index on molecular size Information indices 235 IAC total information index on atomic composition Information indices 236 mean information index on atomic composition Information indices AAC 237 238 IDE IDM mean information content on the distance equality mean information content on the distance magnitude Information indices Information indices 239 240 IDDE mean information content on the distance degree equality Information indices IDDM mean information content on the distance degree magnitude Information indices 241 IDET total information content on the distance equality Information indices 242 243 total information content on the distance magnitude mean information content on the vertex degree equality IDMI Information indices Information indices IVDE 244 245 IVDM mean information content on the vertex degree magnitude Information indices S0K Kier symmetry index Information indices 246 HVcpx graph vertex complexity index Information indices 247 248 HDcpx Uindex graph distance complexity index (log function) Balaban U index Information indices Information indices 249 250 Vindex Balaban V index Information indices Balaban X index Information indices Xindex 251 Information indices Yindex 252 253 IC0 IC1 Information Content index (neighborhood symmetry of 0-order) Information Content index (neighborhood symmetry of 1-order) Information indices Information indices 254 255 IC2 IC3 Information Content index (neighborhood symmetry of 2-order) Information Content index (neighborhood symmetry of 3-order) Information indices Information indices 256 257 IC4 IC5 Information Content index (neighborhood symmetry of 4-order) Information Content index (neighborhood symmetry of 5-order) Information indices Information indices 258 Total Information Content index (neighborhood symmetry of 0-order) TIC0 Information indices 259 TIC1 Total Information Content index (neighborhood symmetry of 1-order) Total Information Content index (neighborhood symmetry of 2-order) Information indices 260 TIC2 Information indices Total Information Content index (neighborhood symmetry of 3-order)
Total Information Content index (neighborhood symmetry of 4-order) 261 TIC3 Information indices 262 TIC4 Information indices 263 Total Information Content index (neighborhood symmetry of 5-order) Information indices Structural Information Content index (neighborhood symmetry of 0-order) Structural Information Content index (neighborhood symmetry of 1-order) 264 SIC0 Information indices 265 SIC1 Information indices 266 267 Structural Information Content index (neighborhood symmetry of 2-order Structural Information Content index (neighborhood symmetry of 3-order SIC2 Information indices SIC3 Information indices 268 SIC4 Structural Information Content index (neighborhood symmetry of 4-order Information indices Structural Information Content index (neighborhood symmetry of 5-order) Complementary Information Content index (neighborhood symmetry of 0-order) 269 SIC5 Information indices 270 CICO Information indices 271 272 CIC1 Complementary Information Content index (neighborhood symmetry of 1-order) Complementary Information Content index (neighborhood symmetry of 2-order) Information indices Information indices 273 CIC3 Complementary Information Content index (neighborhood symmetry of 3-order) Information indices 274 CIC4 Complementary Information Content index (neighborhood symmetry of 4-order) Complementary Information Content index (neighborhood symmetry of 5-order) Information indices 275 CIC5 Information indices Bond Information Content index (neighborhood symmetry of 0-order) Bond Information Content index (neighborhood symmetry of 1-order) 276 BIC0 Information indices 277 BIC1 Information indices 278 279 BIC2 BIC3 Bond Information Content index (neighborhood symmetry of 2-order) Bond Information Content index (neighborhood symmetry of 3-order) Information indices Information indices 280 Bond Information Content index (neighborhood symmetry of 4-order) BIC4 Information indices 281 BIC5 Bond Information Content index (neighborhood symmetry of 5-order) Information indices 282 Balaban-like index from adjacency matrix 2D matrix-based descriptors JA spectral positive sum from adjacency matrix normalized spectral positive sum from adjacency matrix 283 SpPos 2D matrix-based descriptors

2D matrix-based descriptors

SpPosA A



285	SpPosLog A	logarithmic spectral positive sum from adjacency matrix	2D matrix-based descriptors
286	SpMax A	leading eigenvalue from adjacency matrix (Lovasz-Pelikan index)	2D matrix-based descriptors
287	SpMaxA_A	normalized leading eigenvalue from adjacency matrix	2D matrix-based descriptors
288	SpDiam_A	spectral diameter from adjacency matrix	2D matrix-based descriptors
289	SpAD_A	spectral absolute deviation from adjacency matrix	2D matrix-based descriptors
	SpMAD_A	spectral mean absolute deviation from adjacency matrix	2D matrix-based descriptors
291	Ho_A	Hosoya-like index (log function) from adjacency matrix	2D matrix-based descriptors
292	EE_A	Estrada-like index (log function) from adjacency matrix	2D matrix-based descriptors
	VE1_A	coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
	VE2_A	average coefficient of the last eigenvector from adjacency matrix	2D matrix-based descriptors
	VE3_A	logarithmic coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors
	VR1_A	Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors
297 298	VR2_A VR3_A	normalized Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors 2D matrix-based descriptors
	Wi D	logarithmic Randic-like eigenvector-based index from adjacency matrix Wiener-like index from topological distance matrix (Wiener index)	2D matrix-based descriptors
	WiA D	average Wiener-like index from topological distance matrix	2D matrix-based descriptors
301	AVS D	average vertex sum from topological distance matrix	2D matrix-based descriptors
	H D	Harary-like index from topological distance matrix (Harary index)	2D matrix-based descriptors
	Chi D	Randic-like index from topological distance matrix	2D matrix-based descriptors
	ChiA_D	average Randic-like index from topological distance matrix	2D matrix-based descriptors
305	J_D	Balaban-like index from topological distance matrix (Balaban distance connectivity index)	2D matrix-based descriptors
306	HyWi_D	hyper-Wiener-like index (log function) from topological distance matrix	2D matrix-based descriptors
307	SpPos_D	spectral positive sum from topological distance matrix	2D matrix-based descriptors
	SpPosA_D	normalized spectral positive sum from topological distance matrix	2D matrix-based descriptors
309	SpPosLog_D	logarithmic spectral positive sum from topological distance matrix	2D matrix-based descriptors
	SpMax_D	leading eigenvalue from topological distance matrix	2D matrix-based descriptors
311	SpMaxA_D	normalized leading eigenvalue from topological distance matrix	2D matrix-based descriptors
	SpDiam_D	spectral diameter from topological distance matrix	2D matrix-based descriptors
	SpAD_D	spectral absolute deviation from topological distance matrix	2D matrix-based descriptors
314	SpMAD_D	spectral mean absolute deviation from topological distance matrix	2D matrix-based descriptors
	Ho_D	Hosoya-like index (log function) from topological distance matrix	2D matrix-based descriptors
316	EE_D	Estrada-like index (log function) from topological distance matrix	2D matrix-based descriptors
317	SM2_D	spectral moment of order 2 from topological distance matrix	2D matrix-based descriptors
318 319	SM3_D	spectral moment of order 3 from topological distance matrix spectral moment of order 4 from topological distance matrix	2D matrix-based descriptors
	SM4_D SM5_D	spectral moment of order 4 from topological distance matrix spectral moment of order 5 from topological distance matrix	2D matrix-based descriptors 2D matrix-based descriptors
321	SM6 D	· ·	2D matrix-based descriptors
	VE1 D	spectral moment of order 6 from topological distance matrix coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
	VE1_D VE2_D	average coefficient of the last eigenvector from topological distance matrix	2D matrix-based descriptors
	VE3 D	logarithmic coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors
	VR1_D	Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
	VR2 D	normalized Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
	VR3 D	logarithmic Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors
	QW L	quasi-Wiener index (Kirchhoff number) from Laplace matrix	2D matrix-based descriptors
	TI1 L	first Mohar index from Laplace matrix	2D matrix-based descriptors
	TI2 L	second Mohar index from Laplace matrix	2D matrix-based descriptors
331	STN L	spanning tree number (log function) from Laplace matrix	2D matrix-based descriptors
332	SpPos L	spectral positive sum from Laplace matrix	2D matrix-based descriptors
333	SpPosA_L	normalized spectral positive sum from Laplace matrix	2D matrix-based descriptors
334	SpPosLog_L	logarithmic spectral positive sum from Laplace matrix	2D matrix-based descriptors
335	SpMax_L	leading eigenvalue from Laplace matrix	2D matrix-based descriptors
	SpMaxA_L	normalized leading eigenvalue from Laplace matrix	2D matrix-based descriptors
	SpDiam_L	spectral diameter from Laplace matrix	2D matrix-based descriptors
	SpAD_L	spectral absolute deviation from Laplace matrix	2D matrix-based descriptors
	SpMAD_L	spectral mean absolute deviation from Laplace matrix	2D matrix-based descriptors
	Ho_L	Hosoya-like index (log function) from Laplace matrix	2D matrix-based descriptors
341	EE_L	Estrada-like index (log function) from Laplace matrix	2D matrix-based descriptors
	SM2_L	spectral moment of order 2 from Laplace matrix	2D matrix-based descriptors
	SM3_L SM4_L	spectral moment of order 3 from Laplace matrix	2D matrix-based descriptors
345	SM5_L	spectral moment of order 4 from Laplace matrix spectral moment of order 5 from Laplace matrix	2D matrix-based descriptors 2D matrix-based descriptors
346	SM6 L	spectral moment of order 6 from Laplace matrix	2D matrix-based descriptors
347	VE1 L	coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
	VE1_L VE2_L	average coefficient of the last eigenvector from Laplace matrix	2D matrix-based descriptors
349	VE3 L	logarithmic coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors
350	VR1_L	Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
351	VR2_L	normalized Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
352	VR3_L	logarithmic Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors
353	AVS_X	average vertex sum from chi matrix	2D matrix-based descriptors
354	H_X	Harary-like index from chi matrix	2D matrix-based descriptors
355	Chi_X	Randic-like index from chi matrix	2D matrix-based descriptors
356	ChiA_X	average Randic-like index from chi matrix	2D matrix-based descriptors
357	J_X	Balaban-like index from chi matrix	2D matrix-based descriptors
	HyWi_X	hyper-Wiener-like index (log function) from chi matrix	2D matrix-based descriptors
359	SpPos_X	spectral positive sum from chi matrix	2D matrix-based descriptors
	SpPosA_X	normalized spectral positive sum from chi matrix	2D matrix-based descriptors
361 362	SpPosLog_X	logarithmic spectral positive sum from chi matrix	2D matrix-based descriptors 2D matrix-based descriptors
362 363	SpMax_X SpMaxA_X	leading eigenvalue from chi matrix normalized leading eigenvalue from chi matrix	2D matrix-based descriptors 2D matrix-based descriptors
364	SpDiam_X	spectral diameter from chi matrix	2D matrix-based descriptors
365	SpAD_X	spectral absolute deviation from chi matrix	2D matrix-based descriptors
366	SpMAD_X	spectral mean absolute deviation from chi matrix	2D matrix-based descriptors
367	Ho X	Hosoya-like index (log function) from chi matrix	2D matrix-based descriptors
368	EE X	Estrada-like index (log function) from chi matrix	2D matrix-based descriptors
369	SM2_X	spectral moment of order 2 from chi matrix	2D matrix-based descriptors
370	SM3 X	spectral moment of order 3 from chi matrix	2D matrix-based descriptors
371	SM4_X	spectral moment of order 4 from chi matrix	2D matrix-based descriptors
372	SM5_X	spectral moment of order 5 from chi matrix	2D matrix-based descriptors
373	SM6_X	spectral moment of order 6 from chi matrix	2D matrix-based descriptors
374	VE1_X	coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
	VE2_X	average coefficient of the last eigenvector from chi matrix	2D matrix-based descriptors
	VE3_X	logarithmic coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors
	VR1_X	Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
378	VR2_X	normalized Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
	VR3_X	logarithmic Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors
380	Wi_H2	Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors



381	WiA H2	average Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors
382		average vertex sum from reciprocal squared distance matrix	2D matrix-based descriptors
383	Chi_H2	Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
384	ChiA H2	average Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors
385		Balaban-like index from reciprocal squared distance matrix	2D matrix-based descriptors
386	HyWi H2	hyper-Wiener-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
387		spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
388	SpPosA H2	normalized spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
389	SpPosLog_H2	logarithmic spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors
390	SpMax H2	leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
391	SpMaxA_H2	normalized leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors
392	SpDiam H2	spectral diameter from reciprocal squared distance matrix	2D matrix-based descriptors
393	SpAD_H2	spectral absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors
394	SpMAD_H2	spectral mean absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors
395	Ho_H2	Hosoya-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
396	EE_H2	Estrada-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors
397	SM2_H2	spectral moment of order 2 from reciprocal squared distance matrix	2D matrix-based descriptors
398	SM3_H2	spectral moment of order 3 from reciprocal squared distance matrix	2D matrix-based descriptors
399	SM4_H2	spectral moment of order 4 from reciprocal squared distance matrix	2D matrix-based descriptors
400	SM5_H2	spectral moment of order 5 from reciprocal squared distance matrix	2D matrix-based descriptors
401		spectral moment of order 6 from reciprocal squared distance matrix	2D matrix-based descriptors
402	VE1_H2	coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
	VE2_H2	average coefficient of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
	VE3_H2	logarithmic coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors
	VR1_H2	Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
	VR2_H2	normalized Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
407		logarithmic Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors
	Wi_Dt	Wiener-like index from detour matrix (detour index)	2D matrix-based descriptors
409	- '	average Wiener-like index from detour matrix	2D matrix-based descriptors
410	_	average vertex sum from detour matrix	2D matrix-based descriptors
	H_Dt	Harary-like index from detour matrix	2D matrix-based descriptors
	Chi_Dt	Randic-like index from detour matrix	2D matrix-based descriptors
	ChiA_Dt	average Randic-like index from detour matrix	2D matrix-based descriptors
	J_Dt	Balaban-like index from detour matrix	2D matrix-based descriptors
	HyWi_Dt	hyper-Wiener-like index (log function) from detour matrix	2D matrix-based descriptors
	SpPos_Dt	spectral positive sum from detour matrix	2D matrix-based descriptors
417	. –	normalized spectral positive sum from detour matrix	2D matrix-based descriptors
418		logarithmic spectral positive sum from detour matrix	2D matrix-based descriptors
419	. –	leading eigenvalue from detour matrix	2D matrix-based descriptors
420	· –	normalized leading eigenvalue from detour matrix	2D matrix-based descriptors
421	· –	spectral diameter from detour matrix	2D matrix-based descriptors
422 423	. –	spectral absolute deviation from detour matrix	2D matrix-based descriptors
	SpMAD_Dt Ho_Dt	spectral mean absolute deviation from detour matrix	2D matrix-based descriptors
	EE Dt	Hosoya-like index (log function) from detour matrix Estrada like index (log function) from detour matrix	2D matrix-based descriptors
426		Estrada-like index (log function) from detour matrix spectral moment of order 2 from detour matrix	2D matrix-based descriptors 2D matrix-based descriptors
427		spectral moment of order 3 from detour matrix	2D matrix-based descriptors
428		spectral moment of order 4 from detour matrix	2D matrix-based descriptors
429	- ·	spectral moment of order 5 from detour matrix	2D matrix-based descriptors
	SM6 Dt	spectral moment of order 6 from detour matrix	2D matrix-based descriptors
	VE1 Dt	coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
	VE2 Dt	average coefficient of the last eigenvector from detour matrix	2D matrix-based descriptors
	VE3 Dt	logarithmic coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors
	VR1_Dt	Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
	VR2 Dt	normalized Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
	VR3 Dt	logarithmic Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors
	Wi D/Dt	Wiener-like index from distance/detour matrix	2D matrix-based descriptors
438	WiA_D/Dt	average Wiener-like index from distance/detour matrix	2D matrix-based descriptors
439	AVS_D/Dt	average vertex sum from distance/detour matrix	2D matrix-based descriptors
440	H_D/Dt	Harary-like index from distance/detour matrix	2D matrix-based descriptors
441	Chi_D/Dt	Randic-like index from distance/detour matrix	2D matrix-based descriptors
442	ChiA_D/Dt	average Randic-like index from distance/detour matrix	2D matrix-based descriptors
443	J_D/Dt	Balaban-like index from distance/detour matrix	2D matrix-based descriptors
444	HyWi_D/Dt	hyper-Wiener-like index (log function) from distance/detour matrix	2D matrix-based descriptors
445		spectral positive sum from distance/detour matrix	2D matrix-based descriptors
446	SpPosA_D/Dt	normalized spectral positive sum from distance/detour matrix	2D matrix-based descriptors
447	SpPosLog_D/Dt	logarithmic spectral positive sum from distance/detour matrix	2D matrix-based descriptors
448	SpMax_D/Dt	leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
449	SpMaxA_D/Dt	normalized leading eigenvalue from distance/detour matrix	2D matrix-based descriptors
450 451	SpDiam_D/Dt	spectral diameter from distance/detour matrix	2D matrix-based descriptors
451 452	SpAD_D/Dt	spectral absolute deviation from distance/detour matrix	2D matrix-based descriptors
452 453		spectral mean absolute deviation from distance/detour matrix	2D matrix-based descriptors
453 454	Ho_D/Dt EE_D/Dt	Hosoya-like index (log function) from distance/detour matrix Estrada-like index (log function) from distance/detour matrix	2D matrix-based descriptors 2D matrix-based descriptors
454 455	_	spectral moment of order 2 from distance/detour matrix	2D matrix-based descriptors
456	SM3_D/Dt	spectral moment of order 3 from distance/detour matrix	2D matrix-based descriptors
457	SM4 D/Dt	spectral moment of order 4 from distance/detour matrix	2D matrix-based descriptors
458	SM5 D/Dt	spectral moment of order 5 from distance/detour matrix	2D matrix-based descriptors
459	SM6 D/Dt	spectral moment of order 6 from distance/detour matrix	2D matrix-based descriptors
	VE1_D/Dt	coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
461		average coefficient of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
	VE3_D/Dt	logarithmic coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors
	VR1_D/Dt	Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
	VR2_D/Dt	normalized Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
	VR3_D/Dt	logarithmic Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors
466		Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
467		average Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
468	AVS_Dz(Z)	average vertex sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
469		Harary-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
470		Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
471	ChiA_Dz(Z)	average Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
472		Balaban-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors
473	, _ ` /	hyper-Wiener-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors
474	SpAbs_Dz(Z)	graph energy from Barysz matrix weighted by atomic number	2D matrix-based descriptors
475	SpPos_Dz(Z)	spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors
476	SpPosA_Dz(Z)	normalized spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors



SpPosLog_Dz(Z) SpMax_Dz(Z) logarithmic spectral positive sum from Barysz matrix weighted by atomic number leading eigenvalue from Barysz matrix weighted by atomic number 2D matrix-based descriptors 2D matrix-based descriptors 479 SpMaxA_Dz(Z) normalized leading eigenvalue from Barysz matrix weighted by atomic number 2D matrix-based descriptors 480 SpDiam Dz(Z) spectral diameter from Barysz matrix weighted by atomic number 2D matrix-based descriptors 481 SpAD_Dz(Z) spectral absolute deviation from Barysz matrix weighted by atomic number 2D matrix-based descriptors 482 SpMAD Dz(Z)spectral mean absolute deviation from Barysz matrix weighted by atomic number 2D matrix-based descriptors Hosoya-like index (log function) from Barysz matrix weighted by atomic number 2D matrix-based descriptors 483 Ho_Dz(Z) EE_Dz(Z) SM1_Dz(Z) Estrada-like index (log function) from Barysz matrix weighted by atomic number spectral moment of order 1 from Barysz matrix weighted by atomic number 484 2D matrix-based descriptors 2D matrix-based descriptors 485 486 SM2_Dz(Z) spectral moment of order 2 from Barysz matrix weighted by atomic number 2D matrix-based descriptors spectral moment of order 3 from Barysz matrix weighted by atomic number SM3 Dz(Z 487 2D matrix-based descriptors SM4_Dz(Z spectral moment of order 4 from Barysz matrix weighted by atomic number 2D matrix-based descriptors 488 spectral moment of order 5 from Barysz matrix weighted by atomic number spectral moment of order 6 from Barysz matrix weighted by atomic number 489 SM5 Dz(Z 2D matrix-based descriptors 490 $SM6_Dz(Z)$ 2D matrix-based descriptors VE1_Dz(Z) VE2_Dz(Z) coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number average coefficient of the last eigenvector from Barysz matrix weighted by atomic number 491 2D matrix-based descriptors 2D matrix-based descriptors 492 493 VE3_Dz(Z logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number 2D matrix-based descriptors VR1_Dz(Z) VR2_Dz(Z) Randic-like eigenvector-based index from Barysz matrix weighted by atomic number normalized Randic-like eigenvector-based index from Barysz matrix weighted by atomic number 494 2D matrix-based descriptors 2D matrix-based descriptors 495 VR3_Dz(Z) Wi_Dz(m) logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by atomic number Wiener-like index from Barysz matrix weighted by mass 496 2D matrix-based descriptors 2D matrix-based descriptors 497 498 WiA_Dz(m) average Wiener-like index from Barysz matrix weighted by mass 2D matrix-based descriptors average vertex sum from Barysz matrix weighted by mass Harary-like index from Barysz matrix weighted by mass 499 AVS Dz(m) 2D matrix-based descriptors 500 H_Dz(m) 2D matrix-based descriptors Chi_Dz(m) ChiA_Dz(m) Randic-like index from Barysz matrix weighted by mass average Randic-like index from Barysz matrix weighted by mass 501 2D matrix-based descriptors 502 2D matrix-based descriptors Balaban-like index from Barysz matrix weighted by mass hyper-Wiener-like index (log function) from Barysz matrix weighted by mass graph energy from Barysz matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 503 J_Dz(m) HyWi Dz(m) 504 2D matrix-based descriptors 505 SpAbs_Dz(m) SpPos_Dz(m) SpPosA Dz(m) spectral positive sum from Barysz matrix weighted by mass normalized spectral positive sum from Barysz matrix weighted by mass 506 2D matrix-based descriptors 507 2D matrix-based descriptors 508 509 SpPosLog_Dz(m) SpMax_Dz(m) logarithmic spectral positive sum from Barysz matrix weighted by mass leading eigenvalue from Barysz matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 510 SpMaxA_Dz(m) normalized leading eigenvalue from Barysz matrix weighted by mass 2D matrix-based descriptors 511 SpDiam Dz(m) spectral diameter from Barysz matrix weighted by mass spectral absolute deviation from Barysz matrix weighted by mass 2D matrix-based descriptors 512 SpAD_Dz(m) 2D matrix-based descriptors spectral mean absolute deviation from Barysz matrix weighted by mass Hosoya-like index (log function) from Barysz matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 513 SpMAD Dz(m) Ho Dz(m) 514 515 EE_Dz(m) Estrada-like index (log function) from Barysz matrix weighted by mass 2D matrix-based descriptors SM1 Dz(m) spectral moment of order 1 from Barysz matrix weighted by mass spectral moment of order 2 from Barysz matrix weighted by mass 516 2D matrix-based descriptors 517 SM2_Dz(m) 2D matrix-based descriptors 518 519 SM3_Dz(m) SM4_Dz(m) spectral moment of order 3 from Barysz matrix weighted by mass spectral moment of order 4 from Barysz matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 520 SM5_Dz(m spectral moment of order 5 from Barysz matrix weighted by mass 2D matrix-based descriptors spectral moment of order 6 from Barysz matrix weighted by mass coefficient sum of the last eigenvector from Barysz matrix weighted by mass SM6 Dz(m) 521 2D matrix-based descriptors 522 VE1 Dz(m) 2D matrix-based descriptors VE2_Dz(m) VE3_Dz(m) average coefficient of the last eigenvector from Barysz matrix weighted by mass logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by mass 523 2D matrix-based descriptors 524 2D matrix-based descriptors 525 VR1_Dz(m) VR2_Dz(m) Randic-like eigenvector-based index from Barysz matrix weighted by mass normalized Randic-like eigenvector-based index from Barysz matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 526 527 VR3_Dz(m) logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by mass 2D matrix-based descriptors 528 Wi Dz(v) Wiener-like index from Barysz matrix weighted by van der Waals volume average Wiener-like index from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 529 WiA_Dz(v) 2D matrix-based descriptors average vertex sum from Barysz matrix weighted by van der Waals volume Harary-like index from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 530 AVS Dz(v) 531 H_Dz(v) Chi_Dz(v) ChiA Dz(v) 532 Randic-like index from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors average Randic-like index from Barysz matrix weighted by van der Waals volume 533 2D matrix-based descriptors 534 J_Dz(v) Balaban-like index from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 535 HyWi_Dz(v) SpAbs_Dz(v) hyper-Wiener-like index (log function) from Barysz matrix weighted by van der Waals volume graph energy from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 536 2D matrix-based descriptors spectral positive sum from Barysz matrix weighted by van der Waals volume normalized spectral positive sum from Barysz matrix weighted by van der Waals volume 537 SpPos_Dz(v) 2D matrix-based descriptors SpPosA Dz(v) 2D matrix-based descriptors 538 539 SpPosLog_Dz(v) logarithmic spectral positive sum from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors leading eigenvalue from Barysz matrix weighted by van der Waals volume normalized leading eigenvalue from Barysz matrix weighted by van der Waals volume 540 SpMax Dz(v) 2D matrix-based descriptors 541 SpMaxA_Dz(v) 2D matrix-based descriptors 542 SpDiam_Dz(v) SpAD_Dz(v) spectral diameter from Barysz matrix weighted by van der Waals volume spectral absolute deviation from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 543 2D matrix-based descriptors 544 SpMAD_Dz(v) spectral mean absolute deviation from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors Hosoya-like index (log function) from Barysz matrix weighted by van der Waals volume Estrada-like index (log function) from Barysz matrix weighted by van der Waals volume 545 Ho_Dz(v) EE_Dz(v) 2D matrix-based descriptors 546 2D matrix-based descriptors 547 SM1_Dz(v) SM2_Dz(v) spectral moment of order 1 from Barysz matrix weighted by van der Waals volume spectral moment of order 2 from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 548 2D matrix-based descriptors 549 550 SM3_Dz(v) SM4_Dz(v) spectral moment of order 3 from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors spectral moment of order 4 from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors SM5_Dz(v) spectral moment of order 5 from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 551 spectral moment of order 6 from Barysz matrix weighted by van der Waals volume coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume 552 SM6 Dz(v 2D matrix-based descriptors 553 VE1_Dz(v) 2D matrix-based descriptors 554 555 VE2_Dz(v) VE3_Dz(v) average coefficient of the last eigenvector from Barysz matrix weighted by van der Waals volume logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 556 VR1_Dz(v) Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume 2D matrix-based descriptors VR2 Dz(v) normalized Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume 557 2D matrix-based descriptors 558 VR3_Dz(v) 2D matrix-based descriptors 559 560 Wi_Dz(e)
WiA Dz(e) Wiener-like index from Barysz matrix weighted by Sanderson electronegativity average Wiener-like index from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors 561 AVS_Dz(e) average vertex sum from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 562 H_Dz(e) Chi_Dz(e) Harary-like index from Barysz matrix weighted by Sanderson electronegativity Randic-like index from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 563 2D matrix-based descriptors average Randic-like index from Barysz matrix weighted by Sanderson electronegativity Balaban-like index from Barysz matrix weighted by Sanderson electronegativity 564 ChiA_Dz(e) 2D matrix-based descriptors J_Dz(e) 2D matrix-based descriptors 565 566 567 HyWi_Dz(e) SpAbs_Dz(e) hyper-Wiener-like index (log function) from Barysz matrix weighted by Sanderson electronegativity graph energy from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors spectral positive sum from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 568 SpPos_Dz(e) SpPosA_Dz(e) SpPosLog_Dz(e) normalized spectral positive sum from Barysz matrix weighted by Sanderson electronegativity logarithmic spectral positive sum from Barysz matrix weighted by Sanderson electronegativity 569 2D matrix-based descriptors 570 2D matrix-based descriptors SpMax_Dz(e) SpMaxA Dz(e) leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity normalized leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors 571



SpDiam_Dz(e) SpAD_Dz(e) spectral diameter from Barysz matrix weighted by Sanderson electronegativity spectral absolute deviation from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors 574 575 SpMAD Dz(e) spectral mean absolute deviation from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors Ho Dz(e) Hosova-like index (log function) from Barysz matrix weighted by Sanderson electronegativity 576 2D matrix-based descriptors 577 EE_Dz(e) Estrada-like index (log function) from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 578 SM1 Dz(e) spectral moment of order 1 from Barysz matrix weighted by Sanderson electronegativity spectral moment of order 2 from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors 579 SM2_Dz(e) SM3_Dz(e) SM4_Dz(e) spectral moment of order 3 from Barysz matrix weighted by Sanderson electronegativity spectral moment of order 4 from Barysz matrix weighted by Sanderson electronegativity 580 2D matrix-based descriptors 2D matrix-based descriptors 581 582 SM5_Dz(e) spectral moment of order 5 from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors spectral moment of order 6 from Barysz matrix weighted by Sanderson electronegativity coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity SM6 Dz(e 583 2D matrix-based descriptors VE1_Dz(e) 2D matrix-based descriptors 584 VE2_Dz(e) VE3_Dz(e) average coefficient of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity 585 2D matrix-based descriptors 586 2D matrix-based descriptors VR1_Dz(e) VR2_Dz(e) Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity normalized Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity 587 2D matrix-based descriptors 588 2D matrix-based descriptors 589 VR3_Dz(e) logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity 2D matrix-based descriptors Wi_Dz(p) WiA_Dz(p) Wiener-like index from Barysz matrix weighted by polarizability average Wiener-like index from Barysz matrix weighted by polarizability 590 2D matrix-based descriptors 591 2D matrix-based descriptors average vertex sum from Barysz matrix weighted by polarizability Harary-like index from Barysz matrix weighted by polarizability 592 AVS Dz(p 2D matrix-based descriptors 593 2D matrix-based descriptors H Dz(p) 594 Chi_Dz(p) Randic-like index from Barysz matrix weighted by polarizability 2D matrix-based descriptors average Randic-like index from Barysz matrix weighted by polarizability Balaban-like index from Barysz matrix weighted by polarizability 595 ChiA Dz(p) 2D matrix-based descriptors 596 J_Dz(p) 2D matrix-based descriptors hyper-Wiener-like index (log function) from Barysz matrix weighted by polarizability graph energy from Barysz matrix weighted by polarizability HyWi_Dz(p) SpAbs_Dz(p) 597 2D matrix-based descriptors 598 2D matrix-based descriptors SpPos_Dz(p)
SpPosA Dz(p) spectral positive sum from Barysz matrix weighted by polarizability normalized spectral positive sum from Barysz matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 599 600 SpPosLog_Dz(p) logarithmic spectral positive sum from Barysz matrix weighted by polarizability 2D matrix-based descriptors 601 leading eigenvalue from Barysz matrix weighted by polarizability normalized leading eigenvalue from Barysz matrix weighted by polarizability 602 SpMax Dz(p) 2D matrix-based descriptors 603 SpMaxA Dz(p) 2D matrix-based descriptors spectral diameter from Barysz matrix weighted by polarizability spectral absolute deviation from Barysz matrix weighted by polarizability spectral mean absolute deviation from Barysz matrix weighted by polarizability spectral mean absolute deviation from Barysz matrix weighted by polarizability 604 SpDiam_Dz(p) SpAD_Dz(p) 2D matrix-based descriptors 605 2D matrix-based descriptors 606 SpMAD Dz(p) 2D matrix-based descriptors 607 Ho_Dz(p) EE_Dz(p) Hosoya-like index (log function) from Barysz matrix weighted by polarizability Estrada-like index (log function) from Barysz matrix weighted by polarizability 2D matrix-based descriptors 608 2D matrix-based descriptors SM1_Dz(p) SM2_Dz(p) spectral moment of order 1 from Barysz matrix weighted by polarizability spectral moment of order 2 from Barysz matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 609 610 611 SM3_Dz(p) spectral moment of order 3 from Barysz matrix weighted by polarizability 2D matrix-based descriptors SM4 Dz(p) spectral moment of order 4 from Barysz matrix weighted by polarizability 612 2D matrix-based descriptors 613 SM5_Dz(p) spectral moment of order 5 from Barysz matrix weighted by polarizability 2D matrix-based descriptors SM6_Dz(p) spectral moment of order 6 from Barysz matrix weighted by polarizability coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 614 615 616 VE2_Dz(p) average coefficient of the last eigenvector from Barysz matrix weighted by polarizability 2D matrix-based descriptors logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability Randic-like eigenvector-based index from Barysz matrix weighted by polarizability 617 VE3 Dz(p) 2D matrix-based descriptors 618 VR1_Dz(p) 2D matrix-based descriptors normalized Randic-like eigenvector-based index from Barysz matrix weighted by polarizability logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by polarizability VR2_Dz(p) VR3_Dz(p) 619 2D matrix-based descriptors 2D matrix-based descriptors 620 621 Wi_Dz(i) WiA_Dz(i) Wiener-like index from Barysz matrix weighted by ionization potential average Wiener-like index from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 2D matrix-based descriptors 622 623 AVS_Dz(i) average vertex sum from Barysz matrix weighted by ionization potentia 2D matrix-based descriptors 624 H Dz(i) Harary-like index from Barysz matrix weighted by ionization potential Randic-like index from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 625 Chi_Dz(i) 2D matrix-based descriptors 626 627 ChiA Dz(i) average Randic-like index from Barysz matrix weighted by ionization potential Balaban-like index from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 2D matrix-based descriptors J_Dz(i) 628 HyWi_Dz(i) hyper-Wiener-like index (log function) from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 629 SpAbs Dz(i graph energy from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 630 SpPos_Dz(i) spectral positive sum from Barysz matrix weighted by ionization potentia 2D matrix-based descriptors 631 SpPosA_Dz(i) SpPosLog_Dz(i) normalized spectral positive sum from Barysz matrix weighted by ionization potential logarithmic spectral positive sum from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 2D matrix-based descriptors 632 leading eigenvalue from Barysz matrix weighted by ionization potential normalized leading eigenvalue from Barysz matrix weighted by ionization potential 633 SpMax_Dz(i) 2D matrix-based descriptors 2D matrix-based descriptors SpMaxA Dz(i) 634 SpDiam_Dz(i) spectral diameter from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 635 SpAD_Dz(i) SpMAD_Dz(i) spectral absolute deviation from Barysz matrix weighted by ionization potential spectral mean absolute deviation from Barysz matrix weighted by ionization potential 636 2D matrix-based descriptors 637 2D matrix-based descriptors 638 Ho_Dz(i) EE_Dz(i) Hosoya-like index (log function) from Barysz matrix weighted by ionization potential Estrada-like index (log function) from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 2D matrix-based descriptors 639 spectral moment of order 1 from Barysz matrix weighted by ionization potential spectral moment of order 2 from Barysz matrix weighted by ionization potential 640 SM1_Dz(i) 2D matrix-based descriptors 641 SM2 Dz(i) 2D matrix-based descriptors spectral moment of order 3 from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 642 SM3_Dz(i) 643 SM4 Dz(i) spectral moment of order 4 from Barysz matrix weighted by ionization potential spectral moment of order 5 from Barysz matrix weighted by ionization potential 2D matrix-based descriptors SM5 Dz(i) 2D matrix-based descriptors 644 SM6_Dz(i) VE1_Dz(i) 645 spectral moment of order 6 from Barysz matrix weighted by ionization potential 2D matrix-based descriptors coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential average coefficient of the last eigenvector from Barysz matrix weighted by ionization potential 646 2D matrix-based descriptors VE2_Dz(i) 2D matrix-based descriptors 647 VE3_Dz(i) VR1_Dz(i) logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential 648 2D matrix-based descriptors 649 2D matrix-based descriptors VR2_Dz(i) VR3_Dz(i) normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential 2D matrix-based descriptors 2D matrix-based descriptors 650 651 652 Wi_B(m) Wiener-like index from Burden matrix weighted by mass 2D matrix-based descriptors average Wiener-like index from Burden matrix weighted by mass average vertex sum from Burden matrix weighted by mass 653 WiA B(m) 2D matrix-based descriptors AVS_B(m) 2D matrix-based descriptors 654 655 656 Chi_B(m) ChiA_B(m) Randic-like index from Burden matrix weighted by mass average Randic-like index from Burden matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 657 J_B(m) Balaban-like index from Burden matrix weighted by mass 2D matrix-based descriptors HyWi_B(m) hyper-Wiener-like index (log function) from Burden matrix weighted by mass graph energy from Burden matrix weighted by mass 658 2D matrix-based descriptors 659 SpAbs_B(m) 2D matrix-based descriptors spectral positive sum from Burden matrix weighted by mass normalized spectral positive sum from Burden matrix weighted by mass 660 SpPos_B(m) 2D matrix-based descriptors SpPosA_B(m) 2D matrix-based descriptors 661 SpPosLog_B(m) SpMax_B(m) logarithmic spectral positive sum from Burden matrix weighted by mass leading eigenvalue from Burden matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 662 663 SpMaxA_B(m) normalized leading eigenvalue from Burden matrix weighted by mass 2D matrix-based descriptors 664 spectral diameter from Burden matrix weighted by mass spectral absolute deviation from Burden matrix weighted by mass 665 SpDiam B(m) 2D matrix-based descriptors 666 SpAD_B(m) 2D matrix-based descriptors spectral mean absolute deviation from Burden matrix weighted by mass Hosoya-like index (log function) from Burden matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors SpMAD_B(m) 667

Ho B(m)



EE_B(m) SM1_B(m) Estrada-like index (log function) from Burden matrix weighted by mass spectral moment of order 1 from Burden matrix weighted by mass 2D matrix-based descriptors 2D matrix-based descriptors 670 671 SM2 B(m) spectral moment of order 2 from Burden matrix weighted by mass 2D matrix-based descriptors SM3 B(m) spectral moment of order 3 from Burden matrix weighted by mass 672 2D matrix-based descriptors 673 SM4_B(m) spectral moment of order 4 from Burden matrix weighted by mass 2D matrix-based descriptors 674 SM5 B(m) spectral moment of order 5 from Burden matrix weighted by mass 2D matrix-based descriptors spectral moment of order 6 from Burden matrix weighted by mass 2D matrix-based descriptors 675 SM6_B(m) VE1_B(m) VE2_B(m) coefficient sum of the last eigenvector from Burden matrix weighted by mass average coefficient of the last eigenvector from Burden matrix weighted by mass 676 2D matrix-based descriptors 2D matrix-based descriptors 677 logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by mass Randic-like eigenvector-based index from Burden matrix weighted by mass 678 VE3_B(m) 2D matrix-based descriptors VR1 B(m) 679 2D matrix-based descriptors VR2_B(m) normalized Randic-like eigenvector-based index from Burden matrix weighted by mass 2D matrix-based descriptors 680 logarithmic Randic-like eigenvector-based index from Burden matrix weighted by mass Wiener-like index from Burden matrix weighted by van der Waals volume 681 VR3 B(m) 2D matrix-based descriptors 682 Wi_B(v) 2D matrix-based descriptors WiA_B(v) AVS B(v) average Wiener-like index from Burden matrix weighted by van der Waals volume average vertex sum from Burden matrix weighted by van der Waals volume Randic-like index from Burden matrix weighted by van der Waals volume 683 2D matrix-based descriptors 2D matrix-based descriptors 684 685 Chi_B(v) 2D matrix-based descriptors average Randic-like index from Burden matrix weighted by van der Waals volume Balaban-like index from Burden matrix weighted by van der Waals volume 686 ChiA B(v) 2D matrix-based descriptors J_B(v) 2D matrix-based descriptors 687 688 HyWi_B(v) hyper-Wiener-like index (log function) from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors graph energy from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 689 SpAbs B(v) 690 SpPos_B(v) spectral positive sum from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors normalized spectral positive sum from Burden matrix weighted by van der Waals volume logarithmic spectral positive sum from Burden matrix weighted by van der Waals volume 691 SpPosA B(v) 2D matrix-based descriptors 692 SpPosLog_B(v) 2D matrix-based descriptors leading eigenvalue from Burden matrix weighted by van der Waals volume normalized leading eigenvalue from Burden matrix weighted by van der Waals volume 693 SpMax B(v) 2D matrix-based descriptors SpMaxA_B(v) 2D matrix-based descriptors 694 SpDiam_B(v) SpAD B(v) spectral diameter from Burden matrix weighted by van der Waals volume spectral absolute deviation from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 695 696 SpMAD_B(v) spectral mean absolute deviation from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 697 Ho_B(v) EE_B(v) Hosoya-like index (log function) from Burden matrix weighted by van der Waals volume Estrada-like index (log function) from Burden matrix weighted by van der Waals volume 698 2D matrix-based descriptors 699 2D matrix-based descriptors 700 701 SM1_B(v) SM2_B(v) spectral moment of order 1 from Burden matrix weighted by van der Waals volume spectral moment of order 2 from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 702 SM3_B(v) spectral moment of order 3 from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 703 SM4 B(v) spectral moment of order 4 from Burden matrix weighted by van der Waals volume spectral moment of order 5 from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 704 SM5_B(v) 2D matrix-based descriptors SM6_B(v) VE1_B(v) spectral moment of order 6 from Burden matrix weighted by van der Waals volume coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 705 706 707 VE2_B(v) average coefficient of the last eigenvector from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors VE3 B(v) logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume 708 2D matrix-based descriptors 709 VR1_B(v) 2D matrix-based descriptors 710 711 VR2_B(v) VR3_B(v) normalized Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume logarithmic Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume 2D matrix-based descriptors 2D matrix-based descriptors 712 Wi_B(e) Wiener-like index from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors average Wiener-like index from Burden matrix weighted by Sanderson electronegativity average vertex sum from Burden matrix weighted by Sanderson electronegativity 713 WiA B(e) 2D matrix-based descriptors 714 AVS B(e) 2D matrix-based descriptors Randic-like index from Burden matrix weighted by Sanderson electronegativity average Randic-like index from Burden matrix weighted by Sanderson electronegativity 715 Chi B(e) 2D matrix-based descriptors ChiA_B(e) 2D matrix-based descriptors 716 717 718 J_B(e) HyWi_B(e) Balaban-like index from Burden matrix weighted by Sanderson electronegativity hyper-Wiener-like index (log function) from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors 719 720 SpAbs_B(e) graph energy from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors SpPos B(e) spectral positive sum from Burden matrix weighted by Sanderson electronegativity normalized spectral positive sum from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 721 SpPosA_B(e) 2D matrix-based descriptors 722 723 logarithmic spectral positive sum from Burden matrix weighted by Sanderson electronegativity leading eigenvalue from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 2D matrix-based descriptors SpPosLog_B(e) SpMax_B(e) 724 SpMaxA_B(e) normalized leading eigenvalue from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors spectral diameter from Burden matrix weighted by Sanderson electronegativity spectral absolute deviation from Burden matrix weighted by Sanderson electronegativity 725 SpDiam B(e) 2D matrix-based descriptors 726 SpAD_B(e) 2D matrix-based descriptors 727 728 SpMAD B(e) spectral mean absolute deviation from Burden matrix weighted by Sanderson electronegativity Hosoya-like index (log function) from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors Ho_B(e) EE_B(e) 2D matrix-based descriptors Estrada-like index (log function) from Burden matrix weighted by Sanderson electronegativity spectral moment of order 1 from Burden matrix weighted by Sanderson electronegativity 729 2D matrix-based descriptors SM1_B(e) SM2_B(e) 2D matrix-based descriptors 730 731 spectral moment of order 2 from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 732 733 spectral moment of order 3 from Burden matrix weighted by Sanderson electronegativity spectral moment of order 4 from Burden matrix weighted by Sanderson electronegativity SM3 B(e) 2D matrix-based descriptors SM4_B(e) 2D matrix-based descriptors spectral moment of order 5 from Burden matrix weighted by Sanderson electronegativity spectral moment of order 6 from Burden matrix weighted by Sanderson electronegativity spectral moment of order 6 from Burden matrix weighted by Sanderson electronegativity coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity average coefficient of the last eigenvector from Burden matrix weighted by Sanderson electronegativity 734 735 SM5 B(e) 2D matrix-based descriptors SM6_B(e) 2D matrix-based descriptors VE1_B(e) VE2_B(e) 736 2D matrix-based descriptors 737 2D matrix-based descriptors 738 739 logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors VE3_B(e) VR1_B(e) VR2_B(e) Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity normalized Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity 2D matrix-based descriptors 740 2D matrix-based descriptors logarithmic Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity Wiener-like index from Burden matrix weighted by polarizability average Wiener-like index from Burden matrix weighted by polarizability 741 742 VR3_B(e) 2D matrix-based descriptors Wi B(p) 2D matrix-based descriptors 743 WiA_B(p) 2D matrix-based descriptors average vertex sum from Burden matrix weighted by polarizability Randic-like index from Burden matrix weighted by polarizability 744 AVS B(p) 2D matrix-based descriptors 745 Chi_B(p) 2D matrix-based descriptors 746 747 ChiA_B(p) J_B(p) average Randic-like index from Burden matrix weighted by polarizability Balaban-like index from Burden matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 748 HyWi_B(p) hyper-Wiener-like index (log function) from Burden matrix weighted by polarizability 2D matrix-based descriptors SpAbs_B(p) SpPos_B(p) graph energy from Burden matrix weighted by polarizability spectral positive sum from Burden matrix weighted by polarizability 749 2D matrix-based descriptors 750 2D matrix-based descriptors SpPosA_B(p) SpPosLog_B(p) 751 752 normalized spectral positive sum from Burden matrix weighted by polarizability logarithmic spectral positive sum from Burden matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 753 SpMax_B(p) leading eigenvalue from Burden matrix weighted by polarizability 2D matrix-based descriptors 754 SpMaxA B(p) normalized leading eigenvalue from Burden matrix weighted by polarizability spectral diameter from Burden matrix weighted by polarizability 2D matrix-based descriptors 755 SpDiam_B(p) 2D matrix-based descriptors SpAD_B(p) SpMAD_B(p) spectral absolute deviation from Burden matrix weighted by polarizability spectral mean absolute deviation from Burden matrix weighted by polarizability 756 2D matrix-based descriptors 2D matrix-based descriptors 757 758 759 Ho_B(p) EE_B(p) Hosoya-like index (log function) from Burden matrix weighted by polarizability Estrada-like index (log function) from Burden matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors SM1_B(p) spectral moment of order 1 from Burden matrix weighted by polarizability 2D matrix-based descriptors 760 SM2_B(p) 761 spectral moment of order 2 from Burden matrix weighted by polarizability 2D matrix-based descriptors 762 SM3_B(p) spectral moment of order 3 from Burden matrix weighted by polarizability 2D matrix-based descriptors spectral moment of order 4 from Burden matrix weighted by polarizability spectral moment of order 5 from Burden matrix weighted by polarizability 2D matrix-based descriptors 2D matrix-based descriptors 763 SM4_B(p) SM5_B(p)



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SM6_B(p)
VE1_B(p)
                                           spectral moment of order 6 from Burden matrix weighted by polarizability coefficient sum of the last eigenvector from Burden matrix weighted by polarizability
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
766
767
        VE2_B(p)
                                           average coefficient of the last eigenvector from Burden matrix weighted by polarizability
                                                                                                                                                                                                                  2D matrix-based descriptors
        VE3 B(p)
                                           logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by polarizability
768
                                                                                                                                                                                                                  2D matrix-based descriptors
769
        VR1_B(p)
                                           Randic-like eigenvector-based index from Burden matrix weighted by polarizability
                                                                                                                                                                                                                  2D matrix-based descriptors
770
        VR2 B(p)
                                           normalized Randic-like eigenvector-based index from Burden matrix weighted by polarizability
                                                                                                                                                                                                                  2D matrix-based descriptors
         VR3_B(p)
                                           logarithmic Randic-like eigenvector-based index from Burden matrix weighted by polarizability
                                                                                                                                                                                                                  2D matrix-based descriptors
771
772
773
        Wi_B(i)
WiA_B(i)
                                           Wiener-like index from Burden matrix weighted by ionization potential average Wiener-like index from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
774
         AVS_B(i)
                                            average vertex sum from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
775
        Chi B(i)
                                           Randic-like index from Burden matrix weighted by ionization potential average Randic-like index from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
776
        ChiA_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
777
778
                                           Balaban-like index from Burden matrix weighted by ionization potential hyper-Wiener-like index (log function) from Burden matrix weighted by ionization potential
         J B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
         HyWi_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           graph energy from Burden matrix weighted by ionization potential spectral positive sum from Burden matrix weighted by ionization potential normalized spectral positive sum from Burden matrix weighted by ionization potential
779
         SpAbs_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
780
                                                                                                                                                                                                                  2D matrix-based descriptors
         SpPos B(i)
781
         SpPosA_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
        SpPosLog_B(i)
SpMax_B(i)
                                           logarithmic spectral positive sum from Burden matrix weighted by ionization potential leading eigenvalue from Burden matrix weighted by ionization potential
782
                                                                                                                                                                                                                  2D matrix-based descriptors
783
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           normalized leading eigenvalue from Burden matrix weighted by ionization potential spectral diameter from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
784
         SpMaxA B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
785
         SpDiam B(i)
786
         SpAD_B(i)
                                            spectral absolute deviation from Burden matrix weighted by ionization potentia
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           spectral mean absolute deviation from Burden matrix weighted by ionization potential Hosoya-like index (log function) from Burden matrix weighted by ionization potential
787
        SpMAD B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
788
         Ho_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
789
790
        EE_B(i)
SM1_B(i)
                                           Estrada-like index (log function) from Burden matrix weighted by ionization potential spectral moment of order 1 from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
        SM2_B(i)
SM3_B(i)
                                           spectral moment of order 2 from Burden matrix weighted by ionization potential spectral moment of order 3 from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
2D matrix-based descriptors
791
792
         SM4_B(i)
                                           spectral moment of order 4 from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
793
         SM5 B(i)
794
                                           spectral moment of order 5 from Burden matrix weighted by ionization potential spectral moment of order 6 from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
795
         SM6 B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
796
797
        VE1_B(i)
VE2_B(i)
                                           coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential average coefficient of the last eigenvector from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
798
         VE3_B(i)
                                            logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
799
         VR1 B(i)
                                           Randic-like eigenvector-based index from Burden matrix weighted by ionization potential normalized Randic-like eigenvector-based index from Burden matrix weighted by ionization potential
                                                                                                                                                                                                                  2D matrix-based descriptors
800
         VR2_B(i)
                                                                                                                                                                                                                  2D matrix-based descriptors
        VR3_B(i)
Wi_B(s)
                                           logarithmic Randic-like eigenvector-based index from Burden matrix weighted by ionization potential Wiener-like index from Burden matrix weighted by I-State
801
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
802
        WiA_B(s)
AVS_B(s)
803
                                           average Wiener-like index from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           average vertex sum from Burden matrix weighted by I-State Randic-like index from Burden matrix weighted by I-State
804
                                                                                                                                                                                                                  2D matrix-based descriptors
805
         Chi_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
806
807
        ChiA_B(s)
J_B(s)
                                           average Randic-like index from Burden matrix weighted by I-State
Balaban-like index from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors 2D matrix-based descriptors
808
         HyWi_B(s)
                                           hyper-Wiener-like index (log function) from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           graph energy from Burden matrix weighted by I-State spectral positive sum from Burden matrix weighted by I-State
809
         SpAbs B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
810
         SpPos_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           normalized spectral positive sum from Burden matrix weighted by I-State logarithmic spectral positive sum from Burden matrix weighted by I-State
811
         SpPosA B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
         SpPosLog_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
812
813
         SpMax_B(s)
SpMaxA_B(s)
                                           leading eigenvalue from Burden matrix weighted by I-State normalized leading eigenvalue from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
814
815
         SpDiam_B(s)
                                           spectral diameter from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           spectral absolute deviation from Burden matrix weighted by I-State spectral mean absolute deviation from Burden matrix weighted by I-State
816
         SpAD B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
817
         SpMAD_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
        Ho_B(s)
EE_B(s)
                                           Hosoya-like index (log function) from Burden matrix weighted by I-State Estrada-like index (log function) from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors 2D matrix-based descriptors
818
819
820
        SM1_B(s
                                           spectral moment of order 1 from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
        SM2 B(s
                                           spectral moment of order 2 from Burden matrix weighted by I-State
821
                                                                                                                                                                                                                  2D matrix-based descriptors
822
         SM3_B(s)
                                            spectral moment of order 3 from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
823
        SM4 B(s)
                                           spectral moment of order 4 from Burden matrix weighted by I-State spectral moment of order 5 from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
         SM5_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
824
                                           spectral moment of order 6 from Burden matrix weighted by I-State coefficient sum of the last eigenvector from Burden matrix weighted by I-State
825
         SM6_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
                                                                                                                                                                                                                  2D matrix-based descriptors
826
         VE1 B(s)
827
        VE2_B(s)
                                           average coefficient of the last eigenvector from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
                                           logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by I-State Randic-like eigenvector-based index from Burden matrix weighted by I-State
828
         VE3 B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
829
         VR1_B(s)
                                                                                                                                                                                                                  2D matrix-based descriptors
830
        VR2_B(s)
                                           normalized Randic-like eigenvector-based index from Burden matrix weighted by I-State logarithmic Randic-like eigenvector-based index from Burden matrix weighted by I-State
                                                                                                                                                                                                                  2D matrix-based descriptors
         VR3 B(s
                                                                                                                                                                                                                  2D matrix-based descriptors
831
                                           Broto-Moreau autocorrelation of lag 1 (log function) weighted by mass Broto-Moreau autocorrelation of lag 2 (log function) weighted by mass Broto-Moreau autocorrelation of lag 3 (log function) weighted by mass
832
         ATS1m
                                                                                                                                                                                                                  2D autocorrelations
833
        ATS2m
                                                                                                                                                                                                                  2D autocorrelations
834
         ATS3m
                                                                                                                                                                                                                  2D autocorrelations
835
        ATS4m
                                           Broto-Moreau autocorrelation of lag 4 (log function) weighted by mass
Broto-Moreau autocorrelation of lag 5 (log function) weighted by mass
                                                                                                                                                                                                                  2D autocorrelations
        ATS5m
                                                                                                                                                                                                                  2D autocorrelations
836
                                           Broto-Moreau autocorrelation of lag 6 (log function) weighted by mass Broto-Moreau autocorrelation of lag 7 (log function) weighted by mass Broto-Moreau autocorrelation of lag 8 (log function) weighted by mass
837
         ATS6m
                                                                                                                                                                                                                  2D autocorrelations
838
        ATS7m
                                                                                                                                                                                                                  2D autocorrelations
         ATS8m
                                                                                                                                                                                                                  2D autocorrelations
839
                                           Broto-Moreau autocorrelation of lag 1 (log function) weighted by van der Waals volume Broto-Moreau autocorrelation of lag 2 (log function) weighted by van der Waals volume
840
        ATS1v
                                                                                                                                                                                                                  2D autocorrelations
841
        ATS2v
                                                                                                                                                                                                                  2D autocorrelations
                                           Broto-Moreau autocorrelation of lag 3 (log function) weighted by van der Waals volume Broto-Moreau autocorrelation of lag 4 (log function) weighted by van der Waals volume
842
        ATS3v
                                                                                                                                                                                                                  2D autocorrelations
        ATS4v
                                                                                                                                                                                                                  2D autocorrelations
843
844
         ATS5v
                                           Broto-Moreau autocorrelation of lag 5 (log function) weighted by van der Waals volume
                                                                                                                                                                                                                  2D autocorrelations
                                           Broto-Moreau autocorrelation of lag 6 (log function) weighted by van der Waals volume Broto-Moreau autocorrelation of lag 7 (log function) weighted by van der Waals volume
845
        ATS6v
                                                                                                                                                                                                                  2D autocorrelations
                                                                                                                                                                                                                  2D autocorrelations
846
        ATS7v
847
848
         ATS8v
                                           Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume Broto-Moreau autocorrelation of lag 1 (log function) weighted by Sanderson electronegativity
                                                                                                                                                                                                                  2D autocorrelations
        ATS1e
                                                                                                                                                                                                                  2D autocorrelations
849
         ATS2e
                                           Broto-Moreau autocorrelation of lag 2 (log function) weighted by Sanderson electronegativity
                                                                                                                                                                                                                  2D autocorrelations
850
        ATS3e
                                           Broto-Moreau autocorrelation of lag 3 (log function) weighted by Sanderson electronegativity Broto-Moreau autocorrelation of lag 4 (log function) weighted by Sanderson electronegativity
                                                                                                                                                                                                                  2D autocorrelations
851
         ATS4e
                                                                                                                                                                                                                  2D autocorrelations
                                           Broto-Moreau autocorrelation of lag 5 (log function) weighted by Sanderson electronegativity Broto-Moreau autocorrelation of lag 6 (log function) weighted by Sanderson electronegativity
852
        ATS5e
                                                                                                                                                                                                                  2D autocorrelations
        ATS6e
                                                                                                                                                                                                                  2D autocorrelations
853
                                           Broto-Moreau autocorrelation of lag 7 (log function) weighted by Sanderson electronegativity Broto-Moreau autocorrelation of lag 8 (log function) weighted by Sanderson electronegativity
        ATS7e
ATS8e
854
                                                                                                                                                                                                                  2D autocorrelations
855
                                                                                                                                                                                                                  2D autocorrelations
                                           Broto-Moreau autocorrelation of lag 1 (log function) weighted by polarizability Broto-Moreau autocorrelation of lag 2 (log function) weighted by polarizability Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability
                                                                                                                                                                                                                  2D autocorrelations
856
         ATS1p
857
        ATS2n
                                                                                                                                                                                                                  2D autocorrelations
858
        ATS3p
                                                                                                                                                                                                                  2D autocorrelations
         ATS4p
                                           Broto-Moreau autocorrelation of lag 4 (log function) weighted by polarizability Broto-Moreau autocorrelation of lag 5 (log function) weighted by polarizability
859
                                                                                                                                                                                                                  2D autocorrelations
```

2D autocorrelations

860

ATS5p



861	ATS6p	Broto-Moreau autocorrelation of lag 6 (log function) weighted by polarizability	2D autocorrelations
862	ATS7p	Broto-Moreau autocorrelation of lag 7 (log function) weighted by polarizability	2D autocorrelations
863	ATS8p	Broto-Moreau autocorrelation of lag 8 (log function) weighted by polarizability	2D autocorrelations
864	ATS1i		2D autocorrelations
		Broto-Moreau autocorrelation of lag 1 (log function) weighted by ionization potential	
865	ATS2i	Broto-Moreau autocorrelation of lag 2 (log function) weighted by ionization potential	2D autocorrelations
866	ATS3i	Broto-Moreau autocorrelation of lag 3 (log function) weighted by ionization potential	2D autocorrelations
867	ATS4i	Broto-Moreau autocorrelation of lag 4 (log function) weighted by ionization potential	2D autocorrelations
868	ATS5i	Broto-Moreau autocorrelation of lag 5 (log function) weighted by ionization potential	2D autocorrelations
869	ATS6i	Broto-Moreau autocorrelation of lag 6 (log function) weighted by ionization potential	2D autocorrelations
870	ATS7i	Broto-Moreau autocorrelation of lag 7 (log function) weighted by ionization potential	2D autocorrelations
871	ATS8i	Broto-Moreau autocorrelation of lag 8 (log function) weighted by ionization potential	2D autocorrelations
	ATS1s	Broto-Moreau autocorrelation of lag 1 (log function) weighted by I-state	2D autocorrelations
	ATS2s	Broto-Moreau autocorrelation of lag 2 (log function) weighted by I-state	2D autocorrelations
874	ATS3s	Broto-Moreau autocorrelation of lag 3 (log function) weighted by I-state	2D autocorrelations
875	ATS4s	Broto-Moreau autocorrelation of lag 4 (log function) weighted by I-state	2D autocorrelations
876	ATS5s	Broto-Moreau autocorrelation of lag 5 (log function) weighted by I-state	2D autocorrelations
877	ATS6s	Broto-Moreau autocorrelation of lag 6 (log function) weighted by I-state	2D autocorrelations
	ATS7s	Broto-Moreau autocorrelation of lag 7 (log function) weighted by I-state	2D autocorrelations
879	ATS8s	Broto-Moreau autocorrelation of lag 8 (log function) weighted by I-state	2D autocorrelations
880	ATSC1m	Centred Broto-Moreau autocorrelation of lag 1 weighted by mass	2D autocorrelations
881	ATSC2m	Centred Broto-Moreau autocorrelation of lag 2 weighted by mass	2D autocorrelations
882	ATSC3m	Centred Broto-Moreau autocorrelation of lag 3 weighted by mass	2D autocorrelations
883	ATSC4m	Centred Broto-Moreau autocorrelation of lag 4 weighted by mass	2D autocorrelations
884	ATSC5m	Centred Broto-Moreau autocorrelation of lag 5 weighted by mass	2D autocorrelations
885	ATSC6m	Centred Broto-Moreau autocorrelation of lag 6 weighted by mass	2D autocorrelations
886	ATSC7m	Centred Broto-Moreau autocorrelation of lag 7 weighted by mass	2D autocorrelations
887	ATSC8m	Centred Broto-Moreau autocorrelation of lag 8 weighted by mass	2D autocorrelations
888	ATSC1v	Centred Broto-Moreau autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations
889	ATSC2v	Centred Broto-Moreau autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
890	ATSC3v	Centred Broto-Moreau autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
891	ATSC4v	Centred Broto-Moreau autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
892		Centred Broto-Moreau autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
893	ATSC6v	Centred Broto-Moreau autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
894	ATSC7v	Centred Broto-Moreau autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
895	ATSC8v	Centred Broto-Moreau autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
896	ATSC1e	Centred Broto-Moreau autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
897	ATSC2e	Centred Broto-Moreau autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations
898	ATSC3e	Centred Broto-Moreau autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations
899	ATSC4e	Centred Broto-Moreau autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
	ATSC5e	Centred Broto-Moreau autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
901	ATSC6e	Centred Broto-Moreau autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
902	ATSC7e	Centred Broto-Moreau autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
903	ATSC8e	Centred Broto-Moreau autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
904	ATSC1p	Centred Broto-Moreau autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
	ATSC2p	Centred Broto-Moreau autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
906	ATSC3p	Centred Broto-Moreau autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
907	ATSC4p	Centred Broto-Moreau autocorrelation of lag 4 weighted by polarizability	2D autocorrelations
908	ATSC5p	Centred Broto-Moreau autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
909	ATSC6p	Centred Broto-Moreau autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
910	ATSC7p	Centred Broto-Moreau autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
	ATSC8p	Centred Broto-Moreau autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
	ATSC1i	Centred Broto-Moreau autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
	ATSC2i	Centred Broto-Moreau autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
914	ATSC3i	Centred Broto-Moreau autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations
915	ATSC4i	Centred Broto-Moreau autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations
916	ATSC5i	Centred Broto-Moreau autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations
	ATSC6i	Centred Broto-Moreau autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations
	ATSC7i	Centred Broto-Moreau autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
	ATSC8i	Centred Broto-Moreau autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
	ATSC1s	Centred Broto-Moreau autocorrelation of lag 1 weighted by I-state	2D autocorrelations
921	ATSC2s	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state	2D autocorrelations
922	ATSC3s	Centred Broto-Moreau autocorrelation of lag 3 weighted by I-state	2D autocorrelations
923	ATSC4s	Centred Broto-Moreau autocorrelation of lag 4 weighted by I-state	2D autocorrelations
924	ATSC5s	Centred Broto-Moreau autocorrelation of lag 5 weighted by I-state	2D autocorrelations
925	ATSC6s	Centred Broto-Moreau autocorrelation of lag 6 weighted by I-state	2D autocorrelations
926			
	ATSC7s	Centred Broto-Moreau autocorrelation of lag 7 weighted by I-state	2D autocorrelations
927	ATSC8s	Centred Broto-Moreau autocorrelation of lag 8 weighted by I-state	2D autocorrelations
928	MATS1m	Moran autocorrelation of lag 1 weighted by mass	2D autocorrelations
929	MATS2m	Moran autocorrelation of lag 2 weighted by mass	2D autocorrelations
930	MATS3m	Moran autocorrelation of lag 3 weighted by mass	2D autocorrelations
931	MATS4m	Moran autocorrelation of lag 4 weighted by mass	2D autocorrelations
932	MATS5m	Moran autocorrelation of lag 5 weighted by mass	2D autocorrelations
933	MATS6m	Moran autocorrelation of lag 6 weighted by mass	2D autocorrelations
934	MATS7m	Moran autocorrelation of lag 7 weighted by mass	2D autocorrelations
935	MATS8m	Moran autocorrelation of lag 8 weighted by mass	2D autocorrelations
936	MATS1v	Moran autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations
937	MATS2v	Moran autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
938	MATS3v	Moran autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
939	MATS4v	Moran autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
940	MATS5v	Moran autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
941	MATS6v	Moran autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
942	MATS7v	Moran autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
943	MATS8v	Moran autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
944	MATS1e	Moran autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
945	MATS2e	Moran autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations
946	MATS3e	Moran autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations
947	MATS4e	Moran autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
948	MATS5e	Moran autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
949	MATS6e	Moran autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
950	MATS7e	Moran autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
951	MATS8e	Moran autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
952	MATS1p	Moran autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
953	MATS2p	Moran autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
954	•		
	MATS3p	Moran autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
955	MATS4p	Moran autocorrelation of lag 4 weighted by polarizability	2D autocorrelations
956	MATS5p	Moran autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
000			



957	MATS6p	Moran autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
958	MATS7p	Moran autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
959	MATS8p	Moran autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
960	MATS1i	Moran autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
961	MATS2i	Moran autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
962	MATS3i	Moran autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations
963	MATS4i	Moran autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations
964	MATS5i	Moran autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations
965	MATS6i	Moran autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations
966	MATS7i	Moran autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
967	MATS8i	Moran autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
968	MATS1s	Moran autocorrelation of lag 1 weighted by I-state	2D autocorrelations
969	MATS2s	Moran autocorrelation of lag 2 weighted by I-state	2D autocorrelations
970	MATS3s	Moran autocorrelation of lag 3 weighted by I-state	2D autocorrelations
971	MATS4s	Moran autocorrelation of lag 4 weighted by I-state	2D autocorrelations
	MATS5s		2D autocorrelations
973		Moran autocorrelation of lag 5 weighted by I-state	
	MATS6s	Moran autocorrelation of lag 6 weighted by I-state	2D autocorrelations
	MATS7s	Moran autocorrelation of lag 7 weighted by I-state	2D autocorrelations
		Moran autocorrelation of lag 8 weighted by I-state	2D autocorrelations
976	GATS1m	Geary autocorrelation of lag 1 weighted by mass	2D autocorrelations
977	GATS2m	Geary autocorrelation of lag 2 weighted by mass	2D autocorrelations
978	GATS3m	Geary autocorrelation of lag 3 weighted by mass	2D autocorrelations
979	GATS4m	Geary autocorrelation of lag 4 weighted by mass	2D autocorrelations
980	GATS5m	Geary autocorrelation of lag 5 weighted by mass	2D autocorrelations
981	GATS6m	Geary autocorrelation of lag 6 weighted by mass	2D autocorrelations
982	GATS7m	Geary autocorrelation of lag 7 weighted by mass	2D autocorrelations
983	GATS8m	Geary autocorrelation of lag 8 weighted by mass	2D autocorrelations
984	GATS1v	Geary autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations
985	GATS2v	Geary autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations
986	GATS3v	Geary autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations
987	GATS4v	Geary autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations
988	GATS5v	Geary autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations
989	GATS6v	Geary autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations
990	GATS7v	Geary autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations
991	GATS8v	Geary autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations
992	GATS1e		
		Geary autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations
993	GATS2e	Geary autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations
994	GATS3e	Geary autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations
995	GATS4e	Geary autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations
996	GATS5e	Geary autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations
997	GATS6e	Geary autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations
998	GATS7e	Geary autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations
999	GATS8e	Geary autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations
1000	GATS1p	Geary autocorrelation of lag 1 weighted by polarizability	2D autocorrelations
1001	GATS2p	Geary autocorrelation of lag 2 weighted by polarizability	2D autocorrelations
1002	GATS3p	Geary autocorrelation of lag 3 weighted by polarizability	2D autocorrelations
	GATS4p	Geary autocorrelation of lag 4 weighted by polarizability	2D autocorrelations
	GATS5p	Geary autocorrelation of lag 5 weighted by polarizability	2D autocorrelations
	GATS6p	Geary autocorrelation of lag 6 weighted by polarizability	2D autocorrelations
	GATS7p	Geary autocorrelation of lag 7 weighted by polarizability	2D autocorrelations
	GATS8p	Geary autocorrelation of lag 8 weighted by polarizability	2D autocorrelations
	GATS1i	Geary autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
	GATS2i	Geary autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations
	GATS3i		2D autocorrelations
	GATS4i	Geary autocorrelation of lag 3 weighted by ionization potential Geary autocorrelation of lag 4 weighted by ionization potential	
			2D autocorrelations 2D autocorrelations
	GATS5i	Geary autocorrelation of lag 5 weighted by ionization potential	
	GATS6i	Geary autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations
	GATS7i	Geary autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations
	GATS8i	Geary autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations
	GATS1s	Geary autocorrelation of lag 1 weighted by I-state	2D autocorrelations
	GATS2s	Geary autocorrelation of lag 2 weighted by I-state	2D autocorrelations
	GATS3s	Geary autocorrelation of lag 3 weighted by I-state	2D autocorrelations
	GATS4s	Geary autocorrelation of lag 4 weighted by I-state	2D autocorrelations
	GATS5s	Geary autocorrelation of lag 5 weighted by I-state	2D autocorrelations
	GATS6s	Geary autocorrelation of lag 6 weighted by I-state	2D autocorrelations
	GATS7s	Geary autocorrelation of lag 7 weighted by I-state	2D autocorrelations
	GATS8s	Geary autocorrelation of lag 8 weighted by I-state	2D autocorrelations
1024	GGI1	topological charge index of order 1	2D autocorrelations
1025	GGI2	topological charge index of order 2	2D autocorrelations
	GGI3	topological charge index of order 3	2D autocorrelations
	GGI4	topological charge index of order 4	2D autocorrelations
	GGI5	topological charge index of order 5	2D autocorrelations
	GGI6	topological charge index of order 6	2D autocorrelations
	GGI7	topological charge index of order 7	2D autocorrelations
	GGI8	topological charge index of order 8	2D autocorrelations
	GGI9	topological charge index of order 9	2D autocorrelations
	GGI10	topological charge index of order 10	2D autocorrelations
1033		mean topological charge index of order 1	2D autocorrelations
	JGI2	mean topological charge index of order 2	2D autocorrelations
	JGI3		
		mean topological charge index of order 3	2D autocorrelations
	JGI4	mean topological charge index of order 4	2D autocorrelations
	JGI5	mean topological charge index of order 5	2D autocorrelations
	JGI6	mean topological charge index of order 6	2D autocorrelations
1040		mean topological charge index of order 7	2D autocorrelations
	JGI8	mean topological charge index of order 8	2D autocorrelations
	JGI9	mean topological charge index of order 9	2D autocorrelations
	JGI10	mean topological charge index of order 10	2D autocorrelations
1044		global topological charge index	2D autocorrelations
	SpMax1_Bh(m)	largest eigenvalue n. 1 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax2_Bh(m)	largest eigenvalue n. 2 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax3_Bh(m)	largest eigenvalue n. 3 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax4_Bh(m)	largest eigenvalue n. 4 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax5_Bh(m)	largest eigenvalue n. 5 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax6 Bh(m)	largest eigenvalue n. 6 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax7_Bh(m)	largest eigenvalue n. 7 of Burden matrix weighted by mass	Burden eigenvalues
	SpMax8_Bh(m)	largest eigenvalue n. 8 of Burden matrix weighted by mass	Burden eigenvalues
	/	- ,	-



1053 SpMax1_Bh(v) 1054 SpMax2_Bh(v) largest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume largest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume 1055 SpMax3_Bh(v largest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume largest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume largest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume 1056 SpMax4 Bh(v 1057 SpMax5_Bh(v 1058 SpMax6 Bh(v) largest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume largest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume 1059 SpMax7_Bh(v) 1060 SpMax8_Bh(v) 1061 SpMax1_Bh(e) largest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume largest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity 1062 SpMax2_Bh(e) 1063 SpMax3_Bh(e) largest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity largest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity 1064 SpMax4_Bh(e) largest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity 1065 SpMax5_Bh(e) 1066 SpMax6_Bh(e) largest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity largest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity 1067 SpMax7_Bh(e) 1068 SpMax8 Bh(e) largest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity largest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity 1069 SpMax1_Bh(p) largest eigenvalue n. 1 of Burden matrix weighted by polarizability 1070 SpMax2_Bh(p) 1071 SpMax3_Bh(p) largest eigenvalue n. 2 of Burden matrix weighted by polarizability largest eigenvalue n. 3 of Burden matrix weighted by polarizability 1072 SpMax4_Bh(p) 1073 SpMax5_Bh(p) largest eigenvalue n. 4 of Burden matrix weighted by polarizability largest eigenvalue n. 5 of Burden matrix weighted by polarizability 1074 SpMax6_Bh(p) largest eigenvalue n. 6 of Burden matrix weighted by polarizability 1075 SpMax7_Bh(p) 1076 SpMax8_Bh(p) largest eigenvalue n. 7 of Burden matrix weighted by polarizability largest eigenvalue n. 8 of Burden matrix weighted by polarizability 1077 SpMax1_Bh(i) 1078 SpMax2_Bh(i) largest eigenvalue n. 1 of Burden matrix weighted by ionization potential largest eigenvalue n. 2 of Burden matrix weighted by ionization potential 1079 SpMax3_Bh(i) 1080 SpMax4 Bh(i) largest eigenvalue n. 3 of Burden matrix weighted by ionization potential largest eigenvalue n. 4 of Burden matrix weighted by ionization potential SpMax5_Bh(i largest eigenvalue n. 5 of Burden matrix weighted by ionization potential largest eigenvalue n. 6 of Burden matrix weighted by ionization potential largest eigenvalue n. 7 of Burden matrix weighted by ionization potential 1082 SpMax6 Bh(i) 1083 SpMax7_Bh(i) 1084 SpMax8_Bh(i) 1085 SpMax1_Bh(s) largest eigenvalue n. 8 of Burden matrix weighted by ionization potential largest eigenvalue n. 1 of Burden matrix weighted by I-state 1086 SpMax2_Bh(s) largest eigenvalue n. 2 of Burden matrix weighted by I-state 1087 SpMax3_Bh(s) 1088 SpMax4_Bh(s) largest eigenvalue n. 3 of Burden matrix weighted by I-state largest eigenvalue n. 4 of Burden matrix weighted by I-state 1089 SpMax5_Bh(s) 1090 SpMax6_Bh(s) largest eigenvalue n. 5 of Burden matrix weighted by I-state largest eigenvalue n. 6 of Burden matrix weighted by I-state 1091 SpMax7_Bh(s largest eigenvalue n. 7 of Burden matrix weighted by I-state largest eigenvalue n. 8 of Burden matrix weighted by I-state smallest eigenvalue n. 1 of Burden matrix weighted by mass 1092 SpMax8 Bh(s 1093 SpMin1_Bh(m) 1094 SpMin2_Bh(m) 1095 SpMin3_Bh(m) smallest eigenvalue n. 2 of Burden matrix weighted by mass smallest eigenvalue n. 3 of Burden matrix weighted by mass 1096 SpMin4_Bh(m) smallest eigenvalue n. 4 of Burden matrix weighted by mass 1097 SpMin5 Bh(m) smallest eigenvalue n. 5 of Burden matrix weighted by mass 1098 SpMin6_Bh(m) smallest eigenvalue n. 6 of Burden matrix weighted by mass smallest eigenvalue n. 7 of Burden matrix weighted by mass smallest eigenvalue n. 8 of Burden matrix weighted by mass 1099 SpMin7 Bh(m 1100 SpMin8_Bh(m) smallest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume smallest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume 1101 SpMin1_Bh(v) 1102 SpMin2_Bh(v) 1103 SpMin3_Bh(v) smallest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume 1104 SpMin4 Bh(v) smallest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume smallest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume 1105 SpMin5_Bh(v) 1106 SpMin6_Bh(v) 1107 SpMin7_Bh(v) smallest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume smallest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume 1108 SpMin8_Bh(v) smallest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume smallest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity 1109 SpMin1 Bh(e 1110 SpMin2_Bh(e) 1111 SpMin3_Bh(e) 1112 SpMin4_Bh(e) smallest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity 1113 SpMin5_Bh(e) 1114 SpMin6_Bh(e) smallest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity 1115 SpMin7_Bh(e) 1116 SpMin8_Bh(e) 1117 SpMin1_Bh(p) smallest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity smallest eigenvalue n. 1 of Burden matrix weighted by polarizability 1118 SpMin2_Bh(p) 1119 SpMin3_Bh(p) smallest eigenvalue n. 2 of Burden matrix weighted by polarizability smallest eigenvalue n. 3 of Burden matrix weighted by polarizability 1120 SpMin4_Bh(p) 1121 SpMin5 Bh(p) smallest eigenvalue n. 4 of Burden matrix weighted by polarizability smallest eigenvalue n. 5 of Burden matrix weighted by polarizability 1122 SpMin6_Bh(p) smallest eigenvalue n. 6 of Burden matrix weighted by polarizability 1123 SpMin7_Bh(p) 1124 SpMin8 Bh(p) smallest eigenvalue n. 7 of Burden matrix weighted by polarizability smallest eigenvalue n. 8 of Burden matrix weighted by polarizability 1125 SpMin1_Bh(i) 1126 SpMin2_Bh(i) smallest eigenvalue n. 1 of Burden matrix weighted by ionization potential smallest eigenvalue n. 2 of Burden matrix weighted by ionization potential 1127 SpMin3_Bh(i) smallest eigenvalue n. 3 of Burden matrix weighted by ionization potential 1128 SpMin4_Bh(i) 1129 SpMin5_Bh(i) smallest eigenvalue n. 4 of Burden matrix weighted by ionization potential smallest eigenvalue n. 5 of Burden matrix weighted by ionization potential 1130 SpMin6_Bh(i) 1131 SpMin7_Bh(i) smallest eigenvalue n. 6 of Burden matrix weighted by ionization potential smallest eigenvalue n. 7 of Burden matrix weighted by ionization potential 1132 SpMin8_Bh(i) smallest eigenvalue n. 8 of Burden matrix weighted by ionization potential smallest eigenvalue n. 1 of Burden matrix weighted by I-state smallest eigenvalue n. 2 of Burden matrix weighted by I-state 1133 SpMin1 Bh(s) 1134 SpMin2_Bh(s) 1135 SpMin3_Bh(s) 1136 SpMin4 Bh(s) smallest eigenvalue n. 3 of Burden matrix weighted by I-state smallest eigenvalue n. 4 of Burden matrix weighted by I-state 1137 SpMin5_Bh(s smallest eigenvalue n. 5 of Burden matrix weighted by I-state 1138 SpMin6 Bh(s) smallest eigenvalue n. 6 of Burden matrix weighted by I-state smallest eigenvalue n. 7 of Burden matrix weighted by I-state 1139 SpMin7_Bh(s) 1140 SpMin8_Bh(s) 1141 P_VSA_LogP_1 1142 P_VSA_LogP_2 1143 P_VSA_LogP_3 smallest eigenvalue ii. 7 of Burden matrix weighted by I-state
P_VSA-like on LogP, bin 1
P_VSA-like on LogP, bin 2
P_VSA-like on LogP, bin 3 1144 P_VSA_LogP_4 1145 P_VSA_LogP_5 1146 P_VSA_LogP_6 P_VSA-like on LogP, bin 4 P_VSA-like on LogP, bin 5 P_VSA-like on LogP, bin 6 1147 P_VSA_LogP_7 1148 P VSA LogP 8 P_VSA-like on LogP, bin 7 P_VSA-like on LogP, bin 8

Burden eigenvalues P_VSA-like descriptors P_VSA-like descriptors



1149 P_VSA_MR_1	P VSA-like on Molar Refractivity, bin 1	P VSA-like descriptors
1150 P VSA MR 2	P_VSA-like on Molar Refractivity, bin 2	P VSA-like descriptors
1151 P_VSA_MR_3	P_VSA-like on Molar Refractivity, bin 3	P_VSA-like descriptors
	P VSA-like on Molar Refractivity, bin 4	P VSA-like descriptors
1152 P_VSA_MR_4	<u> </u>	
1153 P_VSA_MR_5	P_VSA-like on Molar Refractivity, bin 5	P_VSA-like descriptors
1154 P_VSA_MR_6	P_VSA-like on Molar Refractivity, bin 6	P_VSA-like descriptors
1155 P_VSA_MR_7	P_VSA-like on Molar Refractivity, bin 7	P_VSA-like descriptors
1156 P_VSA_MR_8	P_VSA-like on Molar Refractivity, bin 8	P_VSA-like descriptors
1157 P_VSA_m_1	P VSA-like on mass, bin 1	P_VSA-like descriptors
1158 P_VSA_m_2	P_VSA-like on mass, bin 2	P_VSA-like descriptors
1159 P_VSA_m_3	P_VSA-like on mass, bin 3	P_VSA-like descriptors
1160 P_VSA_m_4	P_VSA-like on mass, bin 4	P_VSA-like descriptors
1161 P_VSA_m_5	P VSA-like on mass, bin 5	P_VSA-like descriptors
1162 P_VSA_v_1	P VSA-like on van der Waals volume, bin 1	P_VSA-like descriptors
	P_VSA-like on van der Waals volume, bin 2	
1163 P_VSA_v_2		P_VSA-like descriptors
1164 P_VSA_v_3	P_VSA-like on van der Waals volume, bin 3	P_VSA-like descriptors
1165 P_VSA_v_4	P_VSA-like on van der Waals volume, bin 4	P_VSA-like descriptors
1166 P_VSA_e_1	P VSA-like on Sanderson electronegativity, bin 1	P VSA-like descriptors
1167 P_VSA_e_2	P_VSA-like on Sanderson electronegativity, bin 2	P VSA-like descriptors
1168 P_VSA_e_3	P_VSA-like on Sanderson electronegativity, bin 3	P_VSA-like descriptors
1169 P_VSA_e_4	P_VSA-like on Sanderson electronegativity, bin 4	P_VSA-like descriptors
1170 P_VSA_e_5	P_VSA-like on Sanderson electronegativity, bin 5	P_VSA-like descriptors
1171 P_VSA_e_6	P VSA-like on Sanderson electronegativity, bin 6	P_VSA-like descriptors
1172 P_VSA_p_1	P_VSA-like on polarizability, bin 1	P_VSA-like descriptors
1173 P_VSA_p_2	P_VSA-like on polarizability, bin 2	P_VSA-like descriptors
1174 P_VSA_p_3	P_VSA-like on polarizability, bin 3	P_VSA-like descriptors
1175 P_VSA_p_4	P_VSA-like on polarizability, bin 4	P_VSA-like descriptors
1176 P_VSA_i_1	P_VSA-like on ionization potential, bin 1	P_VSA-like descriptors
1177 P_VSA_i_2	P_VSA-like on ionization potential, bin 2	P_VSA-like descriptors
1178 P_VSA_i_3	P_VSA-like on ionization potential, bin 3	P_VSA-like descriptors
1179 P_VSA_i_4	P_VSA-like on ionization potential, bin 4	P_VSA-like descriptors
1180 P_VSA_s_1	P_VSA-like on I-state, bin 1	P_VSA-like descriptors
1181 P_VSA_s_2	P_VSA-like on I-state, bin 2	P VSA-like descriptors
1182 P_VSA_s_3	P_VSA-like on I-state, bin 3	P_VSA-like descriptors
1183 P_VSA_s_4	P_VSA-like on I-state, bin 4	P_VSA-like descriptors
1184 P VSA s 5	P_VSA-like on I-state, bin 5	P VSA-like descriptors
1185 P_VSA_s_6	P VSA-like on I-state, bin 6	P VSA-like descriptors
1186 Eta_alpha	eta core count	ETA indices
1187 Eta_alpha_A	eta average core count	ETA indices
1188 Eta epsi	eta electronegativity measure	ETA indices
1189 Eta_epsi_A	eta average electronegativity measure	ETA indices
1190 Eta betaS	eta sigma VEM count	ETA indices
1191 Eta_betaS_A	eta sigma average VEM coun	ETA indices
1192 Eta_betaP	eta pi and lone pair VEM count	ETA indices
1193 Eta betaP A	eta pi and lone pair average VEM count	ETA indices
1194 Eta_beta	eta VEM count	ETA indices
1195 Eta_beta_A	eta average VEM count	ETA indices
1196 Eta_C	eta composite index	ETA indices
1197 Eta_C_A	eta average composite index	ETA indices
1198 Eta L	eta local composite index	ETA indices
1199 Eta L A	eta average local composite index	ETA indices
1200 Eta_F	eta functionality index	ETA indices
1201 Eta_F_A	eta average functionality index	ETA indices
1202 Eta FL	eta local functionality index	ETA indices
1203 Eta_FL_A	eta average local functionality index	ETA indices
	· · · · · · · · · · · · · · · · · · ·	
1204 Eta_B	eta branching index	ETA indices
1205 Eta_B_A	eta average branching index	ETA indices
1206 Eta_sh_p	eta p shape index	ETA indices
1207 Eta_sh_y	eta y shape index	ETA indices
1208 Eta sh x		ETA indices
	eta x shape index	
1209 SpMax_EA	leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1210 SpMaxA_EA	normalized leading eigenvalue from edge adjacency mat.	Edge adjacency indices
1211 SpDiam_EA	spectral diameter from edge adjacency mat.	Edge adjacency indices
1212 SpAD EA	spectral absolute deviation from edge adjacency mat.	Edge adjacency indices
1213 SpMAD_EA	spectral mean absolute deviation from edge adjacency mat.	Edge adjacency indices
1214 SpMax_EA(ed)	leading eigenvalue from edge adjacency mat, weighted by edge degree	Edge adjacency indices
1215 SpMaxA_EA(ed)	normalized leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1216 SpDiam_EA(ed)	spectral diameter from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1217 SpAD_EA(ed)	spectral absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices
1218 SpMAD_EA(ed)	spectral mean absolute deviation from edge adjacency mat, weighted by edge degree	Edge adjacency indices
1219 SpMax_EA(bo)	leading eigenvalue from edge adjacency mat, weighted by bond order	Edge adjacency indices
1220 SpMaxA_EA(bo)	normalized leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices
1221 SpDiam_EA(bo)	spectral diameter from edge adjacency mat. weighted by bond order	Edge adjacency indices
1222 SpAD_EA(bo)		Edge adjacency indices
1223 SpMAD EA(bo)	spectral diameter from edge adjacency mat. weighted by bond order spectral absolute deviation from edge adjacency mat. weighted by bond order	
1224 SpMax EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by bond order	
1227 Opivian_L'A(uiii)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices
100E Callery EA/	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices Edge adjacency indices
1225 SpMaxA_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices Edge adjacency indices Edge adjacency indices
1226 SpDiam_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment	Edge adjacency indices Edge adjacency indices Edge adjacency indices Edge adjacency indices
	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices Edge adjacency indices Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpAD_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ri) 1234 SpMax_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_EA(ed) 1235 SpMaxA_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ri) 1234 SpMax_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_EA(ed) 1236 SpDiam_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMAX_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMaxA_EA(ri) 1234 SpMax_EA(ed) 1235 SpMax_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_EA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_EA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed) 1238 SpMAD_AEA(ed) 1238 SpMAD_AEA(ed) 1238 SpMAD_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed) 1239 SpMax_AEA(bo) 1240 SpMaxA_AEA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute form augmented edge adjacency mat. weighted by edge degree spectral mean absolute form augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by bond order normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed) 1239 SpMax_AEA(bo) 1240 SpMaxA_AEA(bo) 1241 SpDiam_AEA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral absolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_AEA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed) 1239 SpMax_AEA(ed) 1239 SpMax_AEA(ed) 1239 SpMaxA_EA(bo) 1240 SpMaxA_AEA(bo) 1241 SpDiam_AEA(bo) 1242 SpAD_AEA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral basolute deviation from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by fipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral basolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by bond order normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral	Edge adjacency indices
1226 SpDiam_EA(dm) 1227 SpAD_EA(dm) 1228 SpMAD_EA(dm) 1229 SpMax_EA(ri) 1230 SpMaxA_EA(ri) 1231 SpDiam_EA(ri) 1232 SpAD_EA(ri) 1233 SpMAD_EA(ri) 1234 SpMax_AEA(ed) 1235 SpMaxA_EA(ed) 1236 SpDiam_AEA(ed) 1237 SpAD_AEA(ed) 1238 SpMAD_AEA(ed) 1239 SpMaxA_EA(bo) 1240 SpMaxA_AEA(bo) 1241 SpDiam_AEA(bo) 1242 SpAD_AEA(bo) 1243 SpMAA_AEA(bo) 1244 SpDAD_AEA(bo) 1243 SpMAD_AEA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order spectral mean absolute deviation from edge adjacency mat. weighted by bond order leading eigenvalue from edge adjacency mat. weighted by dipole moment normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral diameter from edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment leading eigenvalue from edge adjacency mat. weighted by resonance integral normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral spectral diameter from edge adjacency mat. weighted by resonance integral spectral absolute deviation from edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral leading eigenvalue from augmented edge adjacency mat. weighted by edge degree normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree spectral diameter from augmented edge adjacency mat. weighted by edge degree spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree leading eigenvalue from augmented edge adjacency mat. weighted by bond order normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order spectral diameter from augmented edge adjacency mat. weighted by bond order spectral absolute deviation from augmented edge adjacency mat. weighted by bond order spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond	Edge adjacency indices
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1245 SpMaxA_AEA(dm) 1246 SpDiam_AEA(dm) normalized leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment spectral diameter from augmented edge adjacency mat. weighted by dipole moment 1247 SpAD_AEA(dm) 1248 SpMAD AEA(dm) spectral absolute deviation from augmented edge adjacency mat. weighted by dipole moment spectral mean absolute deviation from augmented edge adjacency mat, weighted by dipole moment 1249 SpMax_AEA(ri) leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral 1250 SpMaxA AEA(ri) normalized leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral spectral diameter from augmented edge adjacency mat. weighted by resonance integral 1251 SpDiam_AEA(ri) 1252 SpAD_AEA(ri) 1253 SpMAD_AEA(ri) spectral absolute deviation from augmented edge adjacency mat. weighted by resonance integral spectral mean absolute deviation from augmented edge adjacency mat. weighted by resonance integral 1254 Chi0_EA connectivity-like index of order 0 from edge adjacency mat. 1255 Chi1 EA connectivity-like index of order 1 from edge adjacency mat. 1256 Chi0_EA(ed) connectivity-like index of order 0 from edge adjacency mat. weighted by edge degree 1257 Chi1_EA(ed) 1258 Chi0_EA(bo) connectivity-like index of order 1 from edge adjacency mat. weighted by edge degree connectivity-like index of order 0 from edge adjacency mat. weighted by bond order 1259 Chi1_EA(bo) 1260 Chi0 EA(dm) connectivity-like index of order 1 from edge adjacency mat. weighted by bond order connectivity-like index of order 0 from edge adjacency mat. weighted by dipole moment 1261 Chi1_EA(dm) connectivity-like index of order 1 from edge adjacency mat. weighted by dipole moment 1262 Chi0_EA(ri) 1263 Chi1_EA(ri) connectivity-like index of order 0 from edge adjacency mat. weighted by resonance integral connectivity-like index of order 1 from edge adjacency mat. weighted by resonance integral 1264 Chi0_AEA(ed) 1265 Chi1_AEA(ed) connectivity-like index of order 0 from augmented edge adjacency mat. weighted by edge degree connectivity-like index of order 1 from augmented edge adjacency mat. weighted by edge degree 1266 Chi0_AEA(bo) connectivity-like index of order 0 from augmented edge adjacency mat. weighted by bond order connectivity-like index of order 1 from augmented edge adjacency mat. weighted by bond order connectivity-like index of order 0 from augmented edge adjacency mat. weighted by dipole moment 1267 Chi1 AEA(bo) 1268 Chi0_AEA(dm) 1269 Chi1_AEA(dm) 1270 Chi0_AEA(ri) connectivity-like index of order 1 from augmented edge adjacency mat. weighted by dipole moment connectivity-like index of order 0 from augmented edge adjacency mat. weighted by resonance integral 1271 Chi1_AEA(ri) 1272 SM02 EA connectivity-like index of order 1 from augmented edge adjacency mat. weighted by resonance integral spectral moment of order 2 from edge adjacency mat. 1273 SM03_EA spectral moment of order 3 from edge adjacency mat spectral moment of order 4 from edge adjacency mat. spectral moment of order 5 from edge adjacency mat. 1274 SM04 EA 1275 SM05 EA 1276 SM06_EA 1277 SM07_EA spectral moment of order 6 from edge adjacency mat spectral moment of order 7 from edge adjacency mat 1278 SM08_EA spectral moment of order 8 from edge adjacency mat 1279 SM09 EA spectral moment of order 9 from edge adjacency mat. spectral moment of order 10 from edge adjacency mat 1280 SM10_EA 1281 SM11_EA 1282 SM12_EA spectral moment of order 11 from edge adjacency mat. spectral moment of order 12 from edge adjacency mat. 1283 SM13_EA spectral moment of order 13 from edge adjacency mat. 1284 SM14 EA spectral moment of order 14 from edge adjacency mat. 1285 SM15_EA spectral moment of order 15 from edge adjacency mat. 1286 SM02_EA(ed) 1287 SM03 EA(ed) spectral moment of order 2 from edge adjacency mat. weighted by edge degree spectral moment of order 3 from edge adjacency mat. weighted by edge degree 1288 SM04_EA(ed) spectral 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mat. weighted by resonance integral

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n. 6 from edge adjacency mat 1404 Eig07_EA 1405 Eig08_EA eigenvalue n. 7 from edge adjacency mat. eigenvalue n. 8 from edge adjacency mat. 1406 Eig09_EA eigenvalue n. 9 from edge adjacency mat. eigenvalue n. 10 from edge adjacency mat 1407 Eig10 EA 1408 Eig11_EA eigenvalue n. 11 from edge adjacency mat. 1409 Eig12_EA 1410 Eig13_EA eigenvalue n. 12 from edge adjacency mat eigenvalue n. 13 from edge adjacency mat 1411 Eig14_EA eigenvalue n. 14 from edge adjacency mat eigenvalue n. 15 from edge adjacency mat 1412 Eig15 EA 1413 Eig01_EA(ed) 1414 Eig02_EA(ed) eigenvalue n. 1 from edge adjacency mat. weighted by edge degree eigenvalue n. 2 from edge adjacency mat. weighted by edge degree 1415 Eig03_EA(ed) eigenvalue n. 3 from edge adjacency mat. weighted by edge degree 1416 Eig04_EA(ed) 1417 Eig05_EA(ed) eigenvalue n. 4 from edge adjacency mat. weighted by edge degree eigenvalue n. 5 from edge adjacency mat. weighted by edge degree 1418 Eig06_EA(ed) 1419 Eig07_EA(ed) eigenvalue n. 6 from 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eigenvalue n. 10 from augmented edge adjacency mat. weighted by edge degree 1482 Eig10_AEA(ed) 1483 Eig11_AEA(ed) 1484 Eig12_AEA(ed) eigenvalue n. 11 from augmented edge adjacency mat. weighted by edge degree eigenvalue n. 12 from augmented edge adjacency mat. weighted by edge degree 1485 Eig13_AEA(ed) 1486 Eig14_AEA(ed) eigenvalue n. 13 from augmented edge adjacency mat. weighted by edge degree eigenvalue n. 14 from augmented edge adjacency mat. weighted by edge degree 1487 Eig15_AEA(ed) eigenvalue n. 15 from augmented edge adjacency mat. weighted by edge degree 1488 Eig01 AEA(bo) eigenvalue n. 1 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 2 from augmented edge adjacency mat. weighted by bond order 1489 Eig02_AEA(bo) 1490 Eig03_AEA(bo) 1491 Eig04_AEA(bo) eigenvalue n. 3 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 4 from augmented edge adjacency mat. weighted by bond order 1492 Eig05_AEA(bo) eigenvalue n. 5 from augmented edge adjacency mat. weighted by bond order 1493 Eig06 AEA(bo) eigenvalue n. 6 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 7 from augmented edge adjacency mat. weighted by bond order 1494 Eig07_AEA(bo) 1495 Eig08_AEA(bo) 1496 Eig09_AEA(bo) eigenvalue n. 8 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 9 from augmented edge adjacency mat. weighted by bond order 1497 Eig10_AEA(bo) eigenvalue n. 10 from augmented edge adjacency mat. weighted by bond order 1498 Eig11_AEA(bo) eigenvalue n. 11 from augmented edge adjacency mat. weighted by bond order 1499 Eig12_AEA(bo) eigenvalue n. 12 from augmented edge adjacency mat. weighted by bond order 1500 Eig13_AEA(bo) 1501 Eig14_AEA(bo) eigenvalue n. 13 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 14 from augmented edge adjacency mat. weighted by bond order 1502 Eig15_AEA(bo) 1503 Eig01_AEA(dm) eigenvalue n. 15 from augmented edge adjacency mat. weighted by bond order eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment 1504 Eig02_AEA(dm) eigenvalue n. 2 from augmented edge adjacency mat. weighted by dipole moment 1505 Eig03 AEA(dm) eigenvalue n. 3 from augmented edge adjacency mat, weighted by dipole moment eigenvalue n. 4 from augmented edge adjacency mat. weighted by dipole moment 1506 Eig04_AEA(dm) 1507 Eig05_AEA(dm) 1508 Eig06 AEA(dm) eigenvalue n. 5 from augmented edge adjacency mat. weighted by dipole moment eigenvalue n. 6 from augmented edge adjacency mat. weighted by dipole moment 1509 Eig07_AEA(dm) 1510 Eig08_AEA(dm) eigenvalue n. 7 from augmented edge adjacency mat. weighted by dipole moment eigenvalue n. 8 from augmented edge adjacency mat. weighted by dipole moment 1511 Eig09_AEA(dm) eigenvalue n. 9 from augmented edge adjacency mat. weighted by dipole moment 1512 Eig10_AEA(dm) 1513 Eig11_AEA(dm) eigenvalue n. 10 from augmented edge adjacency mat. weighted by dipole moment eigenvalue n. 11 from augmented edge adjacency mat. weighted by dipole moment 1514 Eig12_AEA(dm) 1515 Eig13_AEA(dm) eigenvalue n. 12 from augmented edge adjacency mat. weighted by dipole moment eigenvalue n. 13 from augmented edge adjacency mat. weighted by dipole moment 1516 Eig14_AEA(dm) eigenvalue n. 14 from augmented edge adjacency mat. weighted by dipole moment 1517 Eig15_AEA(dm) 1518 Eig01_AEA(ri) eigenvalue n. 15 from augmented edge adjacency mat. weighted by dipole moment eigenvalue n. 1 from augmented edge adjacency mat. weighted by resonance integral 1519 Eig02_AEA(ri) 1520 Eig03 AEA(ri) eigenvalue n. 2 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 3 from augmented edge adjacency mat. weighted by resonance integral 1521 Eig04_AEA(ri eigenvalue n. 4 from augmented edge adjacency mat. weighted by resonance integral 1522 Eig05_AEA(ri) 1523 Eig06_AEA(ri) eigenvalue n. 5 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 6 from augmented edge adjacency mat. weighted by resonance integral 1524 Eig07_AEA(ri) 1525 Eig08_AEA(ri) eigenvalue n. 7 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 8 from augmented edge adjacency mat. weighted by resonance integral 1526 Eig09_AEA(ri) 1527 Eig10_AEA(ri) eigenvalue n. 9 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 10 from augmented edge adjacency mat. weighted by resonance integral 1528 Eig11_AEA(ri) eigenvalue n. 11 from augmented edge adjacency mat. weighted by resonance integra 1529 Eig12_AEA(ri) 1530 Eig13_AEA(ri) eigenvalue n. 12 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 13 from augmented edge adjacency mat. weighted by resonance integral 1531 Eig14_AEA(ri) 1532 Eig15 AEA(ri) eigenvalue n. 14 from augmented edge adjacency mat. weighted by resonance integral eigenvalue n. 15 from augmented edge adjacency mat. weighted by resonance integral Edge adjacency indices Edge adjacency indices
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gravitational index G1 gravitational index G2 (bond-restricted) 1533 G1 Geometrical descriptors 1534 G2 Geometrical descriptors 1535 RGyr radius of gyration (mass weighted) Geometrical descriptors 1536 SPAN span R Geometrical descriptors 1537 SPAM Geometrical descriptors average span R 1538 MEcc molecular eccentricity Geometrical descriptors 1539 SPH spherosity Geometrical descriptors 1540 ASP asphericity Geometrical descriptors 1541 PJI3 Geometrical descriptors 3D Petitjean shape index length-to-breadth ratio by WHIM Harmonic Oscillator Model of Aromaticity index 1542 L/Bw Geometrical descriptors 1543 HOMA Geometrical descriptors 1544 CMBL Geometrical descriptors conjugated maximum bond length aromaticity index HOMA total Geometrical descriptors Geometrical descriptors 1545 ARON 1546 HOMT displacement value / weighted by mass 1547 DISPm Geometrical descriptors 1548 QXXm quadrupole x-component value / weighted by mass Geometrical descriptors 1549 QYYm quadrupole y-component value / weighted by mass Geometrical descriptors quadrupole z-component value / weighted by mass displacement value / weighted by van der Waals volume 1550 QZZm Geometrical descriptors 1551 DISPV Geometrical descriptors quadrupole x-component value / weighted by van der Waals volume quadrupole y-component value / weighted by van der Waals volume quadrupole z-component value / weighted by van der Waals volume 1552 QXXv Geometrical descriptors 1553 QYYv Geometrical descriptors 1554 QZZv Geometrical descriptors displacement value / weighted by Sanderson electronegativity quadrupole x-component value / weighted by Sanderson electronegativity Geometrical descriptors Geometrical descriptors 1555 DISPe 1556 QXXe quadrupole y-component value / weighted by Sanderson electronegativity quadrupole z-component value / weighted by Sanderson electronegativity quadrupole z-component value / weighted by Sanderson electronegativity Geometrical descriptors Geometrical descriptors 1557 QYYe 1558 QZZe 1559 DISPp 1560 QXXp displacement value / weighted by polarizability quadrupole x-component value / weighted by polarizability Geometrical descriptors Geometrical descriptors quadrupole y-component value / weighted by polarizability Geometrical descriptors 1561 QYYp quadrupole z-component value / weighted by polarizability displacement value / weighted by ionization potential 1562 OZZn Geometrical descriptors 1563 DISP Geometrical descriptors 1564 QXXi 1565 QYYi quadrupole x-component value / weighted by ionization potential quadrupole y-component value / weighted by ionization potential Geometrical descriptors Geometrical descriptors 1566 QZZi quadrupole z-component value / weighted by ionization potential Geometrical descriptors 1567 DISPS displacement value / weighted by I-state quadrupole x-component value / weighted by I-state Geometrical descriptors Geometrical descriptors 1568 QXXs quadrupole y-component value / weighted by I-state quadrupole z-component value / weighted by I-state Geometrical descriptors Geometrical descriptors 1569 QYYs 1570 QZZs 1571 Wi_G 1572 WiA_G Wiener-like index from geometrical matrix 3D matrix-based descriptors average Wiener-like index from geometrical matrix 3D matrix-based descriptors 1573 AVS_G average vertex sum from geometrical matrix 3D matrix-based descriptors 1574 H_G 1575 Chi G Harary-like index from geometrical matrix Randic-like index from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1576 ChiA_G average Randic-like index from geometrical matrix 3D matrix-based descriptors 1577 J_G 1578 HyWi_G Balaban-like index from geometrical matrix hyper-Wiener-like index from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1579 SpAbs_G 1580 SpPos_G graph energy from geometrical matrix spectral positive sum from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1581 SpPosA_G 1582 SpPosLog_G normalized spectral positive sum from geometrical matrix logarithmic spectral positive sum from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1583 SpMax_G 1584 SpMaxA_G leading eigenvalue from geometrical matrix 3D matrix-based descriptors normalized leading eigenvalue from geometrical matrix spectral diameter from geometrical matrix 3D matrix-based descriptors 1585 SpDiam_G 3D matrix-based descriptors 1586 SpAD_G 1587 SpMAD_G spectral absolute deviation from geometrical matrix spectral mean absolute deviation from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors Hosoya-like index (log function) from geometrical matrix Estrada-like index (log function) from geometrical matrix spectral moment of order 2 from geometrical matrix 1588 Ho_G 1589 EE G 3D matrix-based descriptors 3D matrix-based descriptors 1590 SM2_G 3D matrix-based descriptors 1591 SM3_G 1592 SM4_G spectral moment of order 3 from geometrical matrix spectral moment of order 4 from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors spectral moment of order 5 from geometrical matrix spectral moment of order 6 from geometrical matrix coefficient sum of the last eigenvector from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1593 SM5 G 1594 SM6 G 1595 VE1_G 3D matrix-based descriptors average coefficient of the last eigenvector from geometrical matrix logarithmic coefficient sum of the last eigenvector from geometrical matrix 1596 VE2 G 3D matrix-based descriptors 1597 VE3_G 3D matrix-based descriptors 1598 VR1 G Randic-like eigenvector-based index from geometrical matrix normalized Randic-like eigenvector-based index from geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1599 VR2_G 1600 VR3_G 1601 Wi RG logarithmic Randic-like eigenvector-based index from geometrical matrix 3D matrix-based descriptors Wiener-like index from reciprocal squared geometrical matrix 3D matrix-based descriptors 1602 WiA_RG average Wiener-like index from reciprocal squared geometrical matrix 3D matrix-based descriptors 1603 AVS RG average vertex sum from reciprocal squared geometrical matrix Harary-like index from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1604 H RG Randic-like index from reciprocal squared geometrical matrix average Randic-like index from reciprocal squared geometrical matrix average Randic-like index from reciprocal squared geometrical matrix Balaban-like index from reciprocal squared geometrical matrix 1605 Chi_RG 1606 ChiA_RG 3D matrix-based descriptors 3D matrix-based descriptors 1607 J_RG 3D matrix-based descriptors 1607 J_RG 1608 HyWi_RG 1609 SpAbs_RG hyper-Wiener-like index from reciprocal squared geometrical matrix graph energy from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1610 SpPos_RG 1611 SpPosA_RG spectral positive sum from reciprocal squared geometrical matrix normalized spectral positive sum from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1612 SpPosLog_RG 1613 SpMax_RG logarithmic spectral positive sum from reciprocal squared geometrical matrix 3D matrix-based descriptors leading eigenvalue from reciprocal squared geometrical matrix normalized leading eigenvalue from reciprocal squared geometrical matrix 3D matrix-based descriptors 1614 SpMaxA_RG 3D matrix-based descriptors 1615 SpDiam_RG 1616 SpAD RG spectral diameter from reciprocal squared geometrical matrix spectral absolute deviation from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1617 SpMAD_RG spectral mean absolute deviation from reciprocal squared geometrical matrix 3D matrix-based descriptors 1618 Ho_RG 1619 EE_RG Hosoya-like index (log function) from reciprocal squared geometrical matrix Estrada-like index (log function) from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1620 SM2_RG 1621 SM3_RG spectral moment of order 2 from reciprocal squared geometrical matrix spectral moment of order 3 from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1622 SM4_RG 1623 SM5_RG spectral moment of order 4 from reciprocal squared geometrical matrix spectral moment of order 5 from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1624 SM6_RG spectral moment of order 6 from reciprocal squared geometrical matrix 3D matrix-based descriptors 1625 VE1 RG coefficient sum of the last eigenvector from reciprocal squared geometrical matrix average coefficient of the last eigenvector from reciprocal squared geometrical matrix 3D matrix-based descriptors 1626 VE2_RG 3D matrix-based descriptors 1627 VE3_RG 1628 VR1 RG logarithmic coefficient sum of the last eigenvector from reciprocal squared geometrical matrix Randic-like eigenvector-based index from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors



1629 VR2_RG 1630 VR3_RG normalized Randic-like eigenvector-based index from reciprocal squared geometrical matrix logarithmic Randic-like eigenvector-based index from reciprocal squared geometrical matrix 3D matrix-based descriptors 3D matrix-based descriptors 1631 Wi_G/D Wiener-like index from distance/distance matrix 3D matrix-based descriptors 1632 WiA G/D average Wiener-like index from distance/distance matrix 3D matrix-based descriptors 1633 AVS_G/D average vertex sum from distance/distance matrix 3D matrix-based descriptors 1634 H G/D Harary-like index from distance/distance matrix 3D matrix-based descriptors 1635 Chi_G/D Randic-like index from distance/distance matrix 3D matrix-based descriptors 1636 ChiA_G/D 1637 J_G/D average Randic-like index from distance/distance matrix Balaban-like index from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors 1638 HyWi_G/D hyper-Wiener-like index from distance/distance matrix 3D matrix-based descriptors graph energy from distance/distance matrix 1639 SpAbs G/D 3D matrix-based descriptors 1640 SpPos_G/D spectral positive sum from distance/distance matrix 3D matrix-based descriptors 1641 SpPosA_G/D 1642 SpPosLog_G/D normalized spectral positive sum from distance/distance matrix logarithmic spectral positive sum from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors 1643 SpMax_G/D 1644 SpMaxA G/D leading eigenvalue from distance/distance matrix normalized leading eigenvalue from distance/distance matrix (folding degree index) 3D matrix-based descriptors 3D matrix-based descriptors 1645 SpDiam_G/D spectral diameter from distance/distance matrix 3D matrix-based descriptors 1646 SpAD_G/D 1647 SpMAD_G/D spectral absolute deviation from distance/distance matrix spectral mean absolute deviation from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors Hosoya-like index (log function) from distance/distance matrix Estrada-like index (log function) from distance/distance matrix 1648 Ho_G/D 1649 EE_G/D 3D matrix-based descriptors 3D matrix-based descriptors 1650 SM2_G/D spectral moment of order 2 from distance/distance matrix 3D matrix-based descriptors 1651 SM3_G/D 1652 SM4_G/D spectral moment of order 3 from distance/distance matrix spectral moment of order 4 from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors 1653 SM5 G/D spectral moment of order 5 from distance/distance matrix spectral moment of order 6 from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors 1654 SM6_G/D 1655 VE1_G/D 1656 VE2 G/D coefficient sum of the last eigenvector from distance/distance matrix average coefficient of the last eigenvector from distance/distance matrix 3D matrix-based descriptors 3D matrix-based descriptors 1657 VE3_G/D logarithmic coefficient sum of the last eigenvector from distance/distance matrix 3D matrix-based descriptors Randic-like eigenvector-based index from distance/distance matrix normalized Randic-like eigenvector-based index from distance/distance matrix 1658 VR1 G/D 3D matrix-based descriptors 1659 VR2 G/D 3D matrix-based descriptors logarithmic Randic-like eigenvector-based index from distance/distance matrix 3D Topological distance based descriptors - lag 1 unweighted 1660 VR3_G/D 1661 TDB01u 3D matrix-based descriptors 3D autocorrelations 1662 TDB02u 3D Topological distance based descriptors - lag 2 unweighted 3D autocorrelations 1663 TDB03u 3D Topological distance based descriptors - lag 3 unweighted 3D Topological distance based descriptors - lag 4 unweighted 3D autocorrelations 3D autocorrelations 1664 TDB04u 1665 TDB05u 1666 TDB06u 3D Topological distance based descriptors - lag 5 unweighted 3D Topological distance based descriptors - lag 6 unweighted 3D autocorrelations 3D autocorrelations 1667 TDB07u 1668 TDB08u 3D Topological distance based descriptors - lag 7 unweighted 3D autocorrelations 3D Topological distance based descriptors - lag 8 unweighted 3D Topological distance based descriptors - lag 9 unweighted 3D autocorrelations 1669 TDB09u 3D autocorrelations 1670 TDB10u 1671 TDB01m 3D Topological distance based descriptors - lag 10 unweighted 3D Topological distance based descriptors - lag 1 weighted by mass 3D autocorrelations 3D autocorrelations 1672 TDB02m 3D Topological distance based descriptors - lag 2 weighted by mass 3D autocorrelations 3D Topological distance based descriptors - lag 3 weighted by mass 3D Topological distance based descriptors - lag 4 weighted by mass 1673 TDB03m 3D autocorrelations 1674 TDB04m 3D autocorrelations 1675 TDB05m 3D Topological distance based descriptors - lag 5 weighted by mass 3D Topological distance based descriptors - lag 6 weighted by mass 3D autocorrelations 1676 TDB06m 3D autocorrelations 1677 TDB07m 1678 TDB08m 3D Topological distance based descriptors - lag 7 weighted by mass 3D Topological distance based descriptors - lag 8 weighted by mass 3D autocorrelations 3D autocorrelations TDB09m 3D Topological distance based descriptors - lag 9 weighted by mass 3D autocorrelations 3D Topological distance based descriptors - lag 10 weighted by mass
3D Topological distance based descriptors - lag 10 weighted by mass
3D Topological distance based descriptors - lag 1 weighted by van der Waals volume 1680 TDB10m 3D autocorrelations 1681 TDB01v 3D autocorrelations 3D Topological distance based descriptors - lag 2 weighted by van der Waals volume 3D Topological distance based descriptors - lag 3 weighted by van der Waals volume 3D autocorrelations 3D autocorrelations 1682 TDB02v 1683 TDB03v 3D Topological distance based descriptors - lag 4 weighted by van der Waals volume 3D Topological distance based descriptors - lag 5 weighted by van der Waals volume 3D Topological distance based descriptors - lag 6 weighted by van der Waals volume 1684 TDB04v 3D autocorrelations 1685 TDB05v 3D autocorrelations 1686 TDB06v 3D autocorrelations 1687 TDB07v 3D Topological distance based descriptors - lag 7 weighted by van der Waals volume 3D Topological distance based descriptors - lag 8 weighted by van der Waals volume 3D autocorrelations TDB08v 3D autocorrelations 1688 1689 TDB09v 1690 TDB10v 3D Topological distance based descriptors - lag 9 weighted by van der Waals volume
3D Topological distance based descriptors - lag 10 weighted by van der Waals volume
3D Topological distance based descriptors - lag 10 weighted by Van der Waals volume
3D Topological distance based descriptors - lag 1 weighted by Sanderson electronegativity 3D autocorrelations 3D autocorrelations 1691 TDB01e 3D autocorrelations 3D Topological distance based descriptors - lag 2 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 3 weighted by Sanderson electronegativity 1692 TDB02e 3D autocorrelations 1693 TDB03e 3D autocorrelations 1694 TDB04e 1695 TDB05e 3D Topological distance based descriptors - lag 4 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 5 weighted by Sanderson electronegativity 3D autocorrelations 3D autocorrelations 3D Topological distance based descriptors - lag 6 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 7 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 8 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 8 weighted by Sanderson electronegativity 1696 TDB06e 1697 TDB07e 3D autocorrelations 3D autocorrelations 1698 TDB08e 3D autocorrelations 1699 TDB09e 3D Topological distance based descriptors - lag 9 weighted by Sanderson electronegativity 3D Topological distance based descriptors - lag 10 weighted by Sanderson electronegativity 3D autocorrelations 1700 TDB10e 3D autocorrelations 3D Topological distance based descriptors - lag 1 weighted by polarizability 3D Topological distance based descriptors - lag 2 weighted by polarizability 3D Topological distance based descriptors - lag 2 weighted by polarizability 3D Topological distance based descriptors - lag 3 weighted by polarizability 1701 TDB01p 1702 TDB02p 3D autocorrelations 3D autocorrelations TDB03p 3D autocorrelations 1703 3D Topological distance based descriptors - lag 4 weighted by polarizability 3D Topological distance based descriptors - lag 5 weighted by polarizability 1704 TDB04p 3D autocorrelations 1705 TDB05p 3D autocorrelations 1706 TDB06p 1707 TDB07p 3D Topological distance based descriptors - lag 6 weighted by polarizability 3D Topological distance based descriptors - lag 7 weighted by polarizability 3D autocorrelations 3D autocorrelations 1708 TDB08p 3D Topological distance based descriptors - lag 8 weighted by polarizability 3D autocorrelations 3D Topological distance based descriptors - lag 9 weighted by polarizability 3D Topological distance based descriptors - lag 10 weighted by polarizability 1709 TDB09n 3D autocorrelations 1710 TDB10p 3D autocorrelations 1711 TDB01i 1712 TDB02i 3D Topological distance based descriptors - lag 1 weighted by ionization potential 3D Topological distance based descriptors - lag 2 weighted by ionization potential 3D autocorrelations 3D autocorrelations 1713 TDB03i 3D Topological distance based descriptors - lag 3 weighted by ionization potential 3D autocorrelations 1714 TDB04 3D Topological distance based descriptors - lag 4 weighted by ionization potential 3D Topological distance based descriptors - lag 5 weighted by ionization potential 3D autocorrelations 1715 TDB05 3D autocorrelations 1716 TDB06i 1717 TDB07i 3D Topological distance based descriptors - lag 6 weighted by ionization potential 3D Topological distance based descriptors - lag 7 weighted by ionization potential 3D autocorrelations 3D autocorrelations 3D Topological distance based descriptors - lag 8 weighted by ionization potential 3D Topological distance based descriptors - lag 9 weighted by ionization potential 1718 TDB08i 1719 TDB09i 3D autocorrelations 3D autocorrelations 1720 TDB10i 3D Topological distance based descriptors - lag 10 weighted by ionization potential 3D autocorrelations 3D Topological distance based descriptors - lag 1 weighted by I-state 3D Topological distance based descriptors - lag 2 weighted by I-state 1721 TDR01s 3D autocorrelations 1722 TDB02s 3D autocorrelations 3D Topological distance based descriptors - lag 3 weighted by I-state 3D Topological distance based descriptors - lag 4 weighted by I-state 1723 TDB03s 3D autocorrelations

3D autocorrelations

1724 TDB04s



1725 TDB05s	3D Topological distance based descriptors - lag 5 weighted by I-state	3D autocorrelations
1726 TDB06s	3D Topological distance based descriptors - lag 6 weighted by I-state	3D autocorrelations
1727 TDB07s	3D Topological distance based descriptors - lag 7 weighted by I-state	3D autocorrelations
1728 TDB08s	3D Topological distance based descriptors - lag 8 weighted by I-state	3D autocorrelations
1729 TDB09s	3D Topological distance based descriptors - lag 9 weighted by I-state	3D autocorrelations
1730 TDB10s	3D Topological distance based descriptors - lag 10 weighted by I-state	3D autocorrelations
1731 TDB01r	3D Topological distance based descriptors - lag 1 weighted by covalent radius	3D autocorrelations
1732 TDB02r	3D Topological distance based descriptors - lag 2 weighted by covalent radius	3D autocorrelations
1733 TDB03r	3D Topological distance based descriptors - lag 3 weighted by covalent radius	3D autocorrelations
1734 TDB04r	3D Topological distance based descriptors - lag 4 weighted by covalent radius	3D autocorrelations
1735 TDB05r	3D Topological distance based descriptors - lag 5 weighted by covalent radius	3D autocorrelations
1736 TDB06r	3D Topological distance based descriptors - lag 6 weighted by covalent radius	3D autocorrelations
1737 TDB07r	3D Topological distance based descriptors - lag 7 weighted by covalent radius	3D autocorrelations
1738 TDB08r	3D Topological distance based descriptors - lag 8 weighted by covalent radius	3D autocorrelations
1739 TDB09r	3D Topological distance based descriptors - lag 9 weighted by covalent radius	3D autocorrelations
1740 TDB10r	3D Topological distance based descriptors - lag 10 weighted by covalent radius	3D autocorrelations
1741 RDF010u	Radial Distribution Function - 010 / unweighted	RDF descriptors
1742 RDF015u	Radial Distribution Function - 015 / unweighted	RDF descriptors
1743 RDF020u	Radial Distribution Function - 020 / unweighted	RDF descriptors
1744 RDF025u	Radial Distribution Function - 025 / unweighted	RDF descriptors
1745 RDF030u	Radial Distribution Function - 030 / unweighted	RDF descriptors
1746 RDF035u	Radial Distribution Function - 035 / unweighted	RDF descriptors
1747 RDF040u	Radial Distribution Function - 040 / unweighted	RDF descriptors
1748 RDF045u	Radial Distribution Function - 045 / unweighted	RDF descriptors
1749 RDF050u	Radial Distribution Function - 050 / unweighted	RDF descriptors
1750 RDF055u	Radial Distribution Function - 055 / unweighted	RDF descriptors
1750 RDF060u	Radial Distribution Function - 060 / unweighted	RDF descriptors
1752 RDF065u	Radial Distribution Function - 065 / unweighted	RDF descriptors
1753 RDF070u	Radial Distribution Function - 070 / unweighted	RDF descriptors
1754 RDF075u	Radial Distribution Function - 075 / unweighted	RDF descriptors
1755 RDF080u	Radial Distribution Function - 080 / unweighted	RDF descriptors
1756 RDF085u 1757 RDF090u	Radial Distribution Function - 085 / unweighted Radial Distribution Function - 090 / unweighted	RDF descriptors
1757 RDF0900 1758 RDF095u	•	RDF descriptors RDF descriptors
	Radial Distribution Function - 095 / unweighted	
1759 RDF100u	Radial Distribution Function - 100 / unweighted	RDF descriptors
1760 RDF105u	Radial Distribution Function - 105 / unweighted	RDF descriptors
1761 RDF110u	Radial Distribution Function - 110 / unweighted	RDF descriptors
1762 RDF115u	Radial Distribution Function - 115 / unweighted	RDF descriptors
1763 RDF120u	Radial Distribution Function - 120 / unweighted	RDF descriptors
1764 RDF125u	Radial Distribution Function - 125 / unweighted	RDF descriptors
1765 RDF130u	Radial Distribution Function - 130 / unweighted	RDF descriptors
1766 RDF135u	Radial Distribution Function - 135 / unweighted	RDF descriptors
1767 RDF140u	Radial Distribution Function - 140 / unweighted	RDF descriptors
1768 RDF145u	Radial Distribution Function - 145 / unweighted	RDF descriptors
1769 RDF150u	Radial Distribution Function - 150 / unweighted	RDF descriptors
1770 RDF155u	Radial Distribution Function - 155 / unweighted	RDF descriptors
1771 RDF010m	Radial Distribution Function - 010 / weighted by mass	RDF descriptors
1772 RDF015m	Radial Distribution Function - 015 / weighted by mass	RDF descriptors
1773 RDF020m	Radial Distribution Function - 020 / weighted by mass	RDF descriptors
1774 RDF025m	Radial Distribution Function - 025 / weighted by mass	RDF descriptors
1775 RDF030m	Radial Distribution Function - 030 / weighted by mass	RDF descriptors
1776 RDF035m	Radial Distribution Function - 035 / weighted by mass	RDF descriptors
1777 RDF040m	Radial Distribution Function - 040 / weighted by mass	RDF descriptors
1778 RDF045m	Radial Distribution Function - 045 / weighted by mass	RDF descriptors
1779 RDF050m	Radial Distribution Function - 050 / weighted by mass	RDF descriptors
1780 RDF055m	Radial Distribution Function - 055 / weighted by mass	RDF descriptors
1781 RDF060m	Radial Distribution Function - 060 / weighted by mass	RDF descriptors
1782 RDF065m	Radial Distribution Function - 065 / weighted by mass	RDF descriptors
1783 RDF070m	Radial Distribution Function - 070 / weighted by mass	RDF descriptors
1784 RDF075m	Radial Distribution Function - 075 / weighted by mass	RDF descriptors
1785 RDF080m	Radial Distribution Function - 080 / weighted by mass	RDF descriptors
1786 RDF085m	Radial Distribution Function - 085 / weighted by mass	RDF descriptors
1787 RDF090m	Radial Distribution Function - 090 / weighted by mass	RDF descriptors
1788 RDF095m	Radial Distribution Function - 095 / weighted by mass	RDF descriptors
1789 RDF100m	Radial Distribution Function - 100 / weighted by mass	RDF descriptors
1790 RDF105m	Radial Distribution Function - 105 / weighted by mass	RDF descriptors
1791 RDF110m	Radial Distribution Function - 110 / weighted by mass	RDF descriptors
1792 RDF115m	Radial Distribution Function - 115 / weighted by mass	RDF descriptors
1793 RDF120m	Radial Distribution Function - 120 / weighted by mass	RDF descriptors
1794 RDF125m	Radial Distribution Function - 125 / weighted by mass	RDF descriptors
1795 RDF130m	Radial Distribution Function - 130 / weighted by mass	RDF descriptors
1796 RDF135m	Radial Distribution Function - 135 / weighted by mass	RDF descriptors
1797 RDF140m	Radial Distribution Function - 140 / weighted by mass	RDF descriptors
1798 RDF145m	Radial Distribution Function - 145 / weighted by mass	RDF descriptors
1799 RDF150m	Radial Distribution Function - 150 / weighted by mass	RDF descriptors
1800 RDF155m	Radial Distribution Function - 155 / weighted by mass	RDF descriptors
1801 RDF010v	Radial Distribution Function - 010 / weighted by van der Waals volume	RDF descriptors
1802 RDF015v	Radial Distribution Function - 015 / weighted by van der Waals volume	RDF descriptors
1803 RDF020v	Radial Distribution Function - 020 / weighted by van der Waals volume	RDF descriptors
1804 RDF025v	Radial Distribution Function - 025 / weighted by van der Waals volume	RDF descriptors
1805 RDF030v	Radial Distribution Function - 030 / weighted by van der Waals volume	RDF descriptors
1806 RDF035v	Radial Distribution Function - 035 / weighted by van der Waals volume	RDF descriptors
1807 RDF040v	Radial Distribution Function - 040 / weighted by van der Waals volume	RDF descriptors
1808 RDF045v	Radial Distribution Function - 045 / weighted by van der Waals volume	RDF descriptors
1809 RDF050v	Radial Distribution Function - 050 / weighted by van der Waals volume	RDF descriptors
1810 RDF055v	Radial Distribution Function - 055 / weighted by van der Waals volume	RDF descriptors
1811 RDF060v	Radial Distribution Function - 060 / weighted by van der Waals volume	RDF descriptors
1812 RDF065v	Radial Distribution Function - 065 / weighted by van der Waals volume	RDF descriptors
1813 RDF070v	Radial Distribution Function - 070 / weighted by van der Waals volume	RDF descriptors
1814 RDF075v	Radial Distribution Function - 075 / weighted by van der Waals volume	RDF descriptors
1815 RDF080v	Radial Distribution Function - 080 / weighted by van der Waals volume	RDF descriptors
		RDF descriptors
1816 RDF085v	Radial Distribution Function - 085 / weighted by van der Waals volume	RDF descriptors RDF descriptors
1816 RDF085v 1817 RDF090v	Radial Distribution Function - 085 / weighted by van der Waals volume Radial Distribution Function - 090 / weighted by van der Waals volume	RDF descriptors
1816 RDF085v 1817 RDF090v 1818 RDF095v	Radial Distribution Function - 085 / weighted by van der Waals volume Radial Distribution Function - 090 / weighted by van der Waals volume Radial Distribution Function - 095 / weighted by van der Waals volume	RDF descriptors RDF descriptors
1816 RDF085v 1817 RDF090v	Radial Distribution Function - 085 / weighted by van der Waals volume Radial Distribution Function - 090 / weighted by van der Waals volume	RDF descriptors



4004	DDE440		DDE 1
	RDF110v		RDF descriptors
	RDF115v		RDF descriptors
1823	RDF120v		RDF descriptors
1824	RDF125v	Radial Distribution Function - 125 / weighted by van der Waals volume	RDF descriptors
1825	RDF130v	Radial Distribution Function - 130 / weighted by van der Waals volume	RDF descriptors
	RDF135v		RDF descriptors
	RDF140v		RDF descriptors
	RDF145v		RDF descriptors
1829	RDF150v	Radial Distribution Function - 150 / weighted by van der Waals volume	RDF descriptors
1830	RDF155v	Radial Distribution Function - 155 / weighted by van der Waals volume	RDF descriptors
1831	RDF010e	Radial Distribution Function - 010 / weighted by Sanderson electronegativity	RDF descriptors
	RDF015e		RDF descriptors
	RDF020e		RDF descriptors
	RDF025e		RDF descriptors
1835	RDF030e		RDF descriptors
1836	RDF035e	Radial Distribution Function - 035 / weighted by Sanderson electronegativity	RDF descriptors
1837	RDF040e	Radial Distribution Function - 040 / weighted by Sanderson electronegativity	RDF descriptors
	RDF045e		RDF descriptors
	RDF050e		RDF descriptors
	RDF055e		RDF descriptors
1841	RDF060e		RDF descriptors
1842	RDF065e	Radial Distribution Function - 065 / weighted by Sanderson electronegativity	RDF descriptors
1843	RDF070e	Radial Distribution Function - 070 / weighted by Sanderson electronegativity	RDF descriptors
	RDF075e		RDF descriptors
	RDF080e		RDF descriptors
	RDF085e		RDF descriptors
1847	RDF090e	Radial Distribution Function - 090 / weighted by Sanderson electronegativity	RDF descriptors
1848	RDF095e	Radial Distribution Function - 095 / weighted by Sanderson electronegativity	RDF descriptors
1849	RDF100e		RDF descriptors
	RDF105e	0 ,	RDF descriptors
			RDF descriptors
	RDF110e		
	RDF115e		RDF descriptors
1853	RDF120e	Radial Distribution Function - 120 / weighted by Sanderson electronegativity	RDF descriptors
1854	RDF125e	Radial Distribution Function - 125 / weighted by Sanderson electronegativity	RDF descriptors
	RDF130e		RDF descriptors
	RDF135e		RDF descriptors
	RDF140e		RDF descriptors
		0 ,	
	RDF145e	0 ,	RDF descriptors
1859	RDF150e	Radial Distribution Function - 150 / weighted by Sanderson electronegativity	RDF descriptors
1860	RDF155e	Radial Distribution Function - 155 / weighted by Sanderson electronegativity	RDF descriptors
1861	RDF010p	Radial Distribution Function - 010 / weighted by polarizability	RDF descriptors
	RDF015p		RDF descriptors
	RDF020p		RDF descriptors
	RDF025p		RDF descriptors
1865	RDF030p	Radial Distribution Function - 030 / weighted by polarizability	RDF descriptors
1866	RDF035p	Radial Distribution Function - 035 / weighted by polarizability	RDF descriptors
1867	RDF040p	Radial Distribution Function - 040 / weighted by polarizability	RDF descriptors
	RDF045p		RDF descriptors
	RDF050p		RDF descriptors
	RDF055p		RDF descriptors
1871	RDF060p	Radial Distribution Function - 060 / weighted by polarizability	RDF descriptors
1872	RDF065p	Radial Distribution Function - 065 / weighted by polarizability	RDF descriptors
1873	RDF070p	Radial Distribution Function - 070 / weighted by polarizability	RDF descriptors
	RDF075p		RDF descriptors
	RDF080p		RDF descriptors
			•
	RDF085p		RDF descriptors
1877	RDF090p	Radial Distribution Function - 090 / weighted by polarizability	RDF descriptors
1878	RDF095p	Radial Distribution Function - 095 / weighted by polarizability	RDF descriptors
1879	RDF100p	Radial Distribution Function - 100 / weighted by polarizability	RDF descriptors
	RDF105p	9 71 7	RDF descriptors
	RDF110p		RDF descriptors
	RDF115p		RDF descriptors
	RDF120p		RDF descriptors
1884	RDF125p		RDF descriptors
1885	RDF130p	Radial Distribution Function - 130 / weighted by polarizability	RDF descriptors
	RDF135p		RDF descriptors
	RDF140p		RDF descriptors
	RDF145p		RDF descriptors
	RDF150p		RDF descriptors
	RDF155p	9 71 7	RDF descriptors
	RDF010i	· ·	RDF descriptors
1892	RDF015i	Radial Distribution Function - 015 / weighted by ionization potential	RDF descriptors
1893	RDF020i		RDF descriptors
	RDF025i		RDF descriptors
	RDF030i	·	RDF descriptors
			TAL ACSCRIPTORS
	RDF035i	Radial Distribution Function - 035 / weighted by ionization potential	RDF descriptors
1898	RDF035i RDF040i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential	RDF descriptors RDF descriptors
4000	RDF035i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential	RDF descriptors
1899	RDF035i RDF040i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential	RDF descriptors RDF descriptors
	RDF035i RDF040i RDF045i RDF050i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900	RDF035i RDF040i RDF045i RDF050i RDF055i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF065i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902 1903	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF066i RDF070i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 066 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902 1903	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF065i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 066 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902 1903 1904	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF066i RDF070i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905	RDF035i RDF040i RDF045i RDF050i RDF055i RDF066i RDF066i RDF070i RDF075i RDF080i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential	RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF066i RDF070i RDF0775i RDF075i RDF080i RDF085i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF066i RDF070i RDF075i RDF080i RDF088i RDF090i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF065i RDF070i RDF075i RDF080i RDF0885i RDF0985i RDF0990i RDF095i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 067 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909	RDF035i RDF040i RDF045i RDF050i RDF055i RDF065i RDF065i RDF070i RDF075i RDF080i RDF080i RDF090i RDF0995i RDF100i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF065i RDF070i RDF075i RDF080i RDF0885i RDF0985i RDF0990i RDF095i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910	RDF035i RDF040i RDF045i RDF050i RDF055i RDF065i RDF065i RDF070i RDF075i RDF080i RDF080i RDF090i RDF0995i RDF100i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 046 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 066 / weighted by ionization potential Radial Distribution Function - 076 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 087 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 1096 / weighted by ionization potential Radial Distribution Function - 1096 / weighted by ionization potential Radial Distribution Function - 1097 / weighted by ionization potential Radial Distribution Function - 1097 / weighted by ionization potential Radial Distribution Function - 1097 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910	RDF035i RDF040i RDF045i RDF055i RDF055i RDF066i RDF076i RDF0770i RDF078i RDF080i RDF080i RDF090i RDF0995i RDF100i RDF100i RDF110i RDF110i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911	RDF035i RDF040i RDF045i RDF055i RDF055i RDF065i RDF065i RDF070i RDF075i RDF080i RDF088i RDF090i RDF090i RDF1090i RDF100i RDF105i RDF115i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 105 / weighted by ionization potential Radial Distribution Function - 115 / weighted by ionization potential Radial Distribution Function - 115 / weighted by ionization potential Radial Distribution Function - 115 / weighted by ionization potential	RDF descriptors RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913	RDF035i RDF040i RDF045i RDF050i RDF055i RDF060i RDF066i RDF075i RDF0775i RDF085i RDF080i RDF090i RDF090i RDF1090i RDF105i RDF105i RDF110i RDF115i RDF115i RDF120i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 046 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 065 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 090 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 105 / weighted by ionization potential Radial Distribution Function - 105 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential	RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914	RDF035i RDF040i RDF045i RDF055i RDF055i RDF060i RDF076i RDF0775i RDF0775i RDF080i RDF085i RDF090i RDF095i RDF105i RDF110i RDF115i RDF1115i RDF115i RDF115i RDF115i RDF115i RDF115i RDF125i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 070 / weighted by ionization potential Radial Distribution Function - 077 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 105 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential	RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914 1915	RDF035i RDF040i RDF045i RDF055i RDF055i RDF065i RDF065i RDF070i RDF0775i RDF080i RDF090i RDF090i RDF1090i RDF105i RDF105i RDF115i RDF115i RDF115i RDF115i RDF115i RDF1126i RDF126i RDF126i RDF130i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 066 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 115 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 125 / weighted by ionization potential Radial Distribution Function - 125 / weighted by ionization potential	RDF descriptors
1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914 1915	RDF035i RDF040i RDF045i RDF055i RDF055i RDF060i RDF076i RDF0775i RDF0775i RDF080i RDF085i RDF090i RDF095i RDF105i RDF110i RDF115i RDF1115i RDF115i RDF115i RDF115i RDF115i RDF115i RDF125i	Radial Distribution Function - 035 / weighted by ionization potential Radial Distribution Function - 040 / weighted by ionization potential Radial Distribution Function - 045 / weighted by ionization potential Radial Distribution Function - 050 / weighted by ionization potential Radial Distribution Function - 055 / weighted by ionization potential Radial Distribution Function - 060 / weighted by ionization potential Radial Distribution Function - 066 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 075 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 080 / weighted by ionization potential Radial Distribution Function - 085 / weighted by ionization potential Radial Distribution Function - 095 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 100 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 110 / weighted by ionization potential Radial Distribution Function - 115 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 120 / weighted by ionization potential Radial Distribution Function - 125 / weighted by ionization potential Radial Distribution Function - 125 / weighted by ionization potential	RDF descriptors



1917	RDF140i	Radial Distribution Function - 140 / weighted by ionization potential	RDF descriptors
		Radial Distribution Function - 145 / weighted by ionization potential	RDF descriptors
		Radial Distribution Function - 150 / weighted by ionization potential	RDF descriptors
		Radial Distribution Function - 155 / weighted by ionization potential	RDF descriptors
		Radial Distribution Function - 010 / weighted by I-state	RDF descriptors
1922		Radial Distribution Function - 015 / weighted by I-state	RDF descriptors
1923	RDF020s	Radial Distribution Function - 020 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 025 / weighted by I-state	RDF descriptors
1925	RDF030s	Radial Distribution Function - 030 / weighted by I-state	RDF descriptors
1926	RDF035s	Radial Distribution Function - 035 / weighted by I-state	RDF descriptors
1927	RDF040s	Radial Distribution Function - 040 / weighted by I-state	RDF descriptors
1928	RDF045s	Radial Distribution Function - 045 / weighted by I-state	RDF descriptors
1929	RDF050s	Radial Distribution Function - 050 / weighted by I-state	RDF descriptors
1930	RDF055s	Radial Distribution Function - 055 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 060 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 065 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 070 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 075 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 080 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 085 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 090 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 095 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 100 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 105 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 110 / weighted by I-state	RDF descriptors RDF descriptors
		Radial Distribution Function - 115 / weighted by I-state Radial Distribution Function - 120 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 125 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 130 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 135 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 140 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 145 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 150 / weighted by I-state	RDF descriptors
		Radial Distribution Function - 155 / weighted by I-state	RDF descriptors
1951	Mor01u	signal 01 / unweighted	3D-MoRSE descriptors
		signal 02 / unweighted	3D-MoRSE descriptors
		signal 03 / unweighted	3D-MoRSE descriptors
		signal 04 / unweighted	3D-MoRSE descriptors
		signal 05 / unweighted	3D-MoRSE descriptors
		signal 06 / unweighted	3D-MoRSE descriptors
		signal 07 / unweighted	3D-MoRSE descriptors
		signal 08 / unweighted	3D-MoRSE descriptors
		signal 09 / unweighted	3D-MoRSE descriptors
		signal 10 / unweighted	3D-MoRSE descriptors
		signal 11 / unweighted	3D-MoRSE descriptors
		signal 12 / unweighted signal 13 / unweighted	3D-MoRSE descriptors 3D-MoRSE descriptors
		signal 14 / unweighted	3D-MoRSE descriptors
		signal 15 / unweighted	3D-MoRSE descriptors
		signal 16 / unweighted	3D-MoRSE descriptors
		signal 17 / unweighted	3D-MoRSE descriptors
1968	Mor18u	signal 18 / unweighted	3D-MoRSE descriptors
		signal 19 / unweighted	3D-MoRSE descriptors
		signal 20 / unweighted	3D-MoRSE descriptors
		signal 21 / unweighted	3D-MoRSE descriptors
		signal 22 / unweighted	3D-MoRSE descriptors
		signal 23 / unweighted signal 24 / unweighted	3D-MoRSE descriptors
		signal 25 / unweighted	3D-MoRSE descriptors 3D-MoRSE descriptors
		signal 26 / unweighted	3D-MoRSE descriptors
		signal 27 / unweighted	3D-MoRSE descriptors
	Mor28u	signal 28 / unweighted	3D-MoRSE descriptors
		signal 29 / unweighted	3D-MoRSE descriptors
		signal 30 / unweighted	3D-MoRSE descriptors
		signal 31 / unweighted	3D-MoRSE descriptors
1982	Mor32u	signal 32 / unweighted	3D-MoRSE descriptors
1983		signal 01 / weighted by mass	3D-MoRSE descriptors
		signal 02 / weighted by mass	3D-MoRSE descriptors
		signal 03 / weighted by mass	3D-MoRSE descriptors
		signal 04 / weighted by mass	3D-MoRSE descriptors
		signal 05 / weighted by mass	3D-MoRSE descriptors
		signal 06 / weighted by mass	3D-MoRSE descriptors
		signal 07 / weighted by mass	3D-MoRSE descriptors
		signal 08 / weighted by mass	3D-MoRSE descriptors
		signal 10 / weighted by mass	3D-MoRSE descriptors
		signal 10 / weighted by mass signal 11 / weighted by mass	3D-MoRSE descriptors 3D-MoRSE descriptors
		signal 17 / weighted by mass	3D-MoRSE descriptors
		signal 13 / weighted by mass	3D-MoRSE descriptors
		signal 14 / weighted by mass	3D-MoRSE descriptors
		signal 15 / weighted by mass	3D-MoRSE descriptors
		signal 16 / weighted by mass	3D-MoRSE descriptors
1999	Mor17m	signal 17 / weighted by mass	3D-MoRSE descriptors
		signal 18 / weighted by mass	3D-MoRSE descriptors
		signal 19 / weighted by mass	3D-MoRSE descriptors
		signal 20 / weighted by mass	3D-MoRSE descriptors
		signal 21 / weighted by mass	3D-MoRSE descriptors
		signal 22 / weighted by mass	3D-MoRSE descriptors
		signal 23 / weighted by mass	3D-MoRSE descriptors
		signal 24 / weighted by mass	3D-MoRSE descriptors
		signal 25 / weighted by mass signal 26 / weighted by mass	3D-MoRSE descriptors 3D-MoRSE descriptors
		signal 27 / weighted by mass	3D-MoRSE descriptors
		signal 28 / weighted by mass	3D-MoRSE descriptors
		signal 29 / weighted by mass	3D-MoRSE descriptors
		signal 30 / weighted by mass	3D-MoRSE descriptors



2013 Mor31m	signal 31 / weighted by mass	3D-MoRSE descriptors
2014 Mor32m	signal 32 / weighted by mass	3D-MoRSE descriptors
2015 Mor01v	signal 01 / weighted by van der Waals volume	3D-MoRSE descriptors
2016 Mor02v	signal 02 / weighted by van der Waals volume	3D-MoRSE descriptors
2017 Mor03v	signal 03 / weighted by van der Waals volume	3D-MoRSE descriptors
2018 Mor04v	signal 04 / weighted by van der Waals volume	3D-MoRSE descriptors
2019 Mor05v	signal 05 / weighted by van der Waals volume	3D-MoRSE descriptors
2020 Mor06v	signal 06 / weighted by van der Waals volume	3D-MoRSE descriptors
2021 Mor07v	signal 07 / weighted by van der Waals volume	3D-MoRSE descriptors
2022 Mor08v	signal 08 / weighted by van der Waals volume	3D-MoRSE descriptors
2023 Mor09v	signal 09 / weighted by van der Waals volume	3D-MoRSE descriptors
2024 Mor10v	signal 10 / weighted by van der Waals volume	3D-MoRSE descriptors
2025 Mor11v	signal 11 / weighted by van der Waals volume	3D-MoRSE descriptors
2026 Mor12v	signal 12 / weighted by van der Waals volume	3D-MoRSE descriptors
2027 Mor13v	signal 13 / weighted by van der Waals volume	3D-MoRSE descriptors
2028 Mor14v	signal 14 / weighted by van der Waals volume	3D-MoRSE descriptors
2029 Mor15v	signal 15 / weighted by van der Waals volume	3D-MoRSE descriptors
2030 Mor16v	signal 16 / weighted by van der Waals volume	3D-MoRSE descriptors
2031 Mor17v	signal 17 / weighted by van der Waals volume	3D-MoRSE descriptors
2032 Mor18v	signal 18 / weighted by van der Waals volume	3D-MoRSE descriptors
2032 Mor19v		
	signal 19 / weighted by van der Waals volume	3D-MoRSE descriptors
2034 Mor20v	signal 20 / weighted by van der Waals volume	3D-MoRSE descriptors
2035 Mor21v	signal 21 / weighted by van der Waals volume	3D-MoRSE descriptors
2036 Mor22v	signal 22 / weighted by van der Waals volume	3D-MoRSE descriptors
2037 Mor23v	signal 23 / weighted by van der Waals volume	3D-MoRSE descriptors
2038 Mor24v	signal 24 / weighted by van der Waals volume	3D-MoRSE descriptors
2039 Mor25v	signal 25 / weighted by van der Waals volume	3D-MoRSE descriptors
2040 Mor26v	signal 26 / weighted by van der Waals volume	3D-MoRSE descriptors
2041 Mor27v	signal 27 / weighted by van der Waals volume	3D-MoRSE descriptors
2042 Mor28v	signal 28 / weighted by van der Waals volume	3D-MoRSE descriptors
2043 Mor29v	signal 29 / weighted by van der Waals volume	3D-MoRSE descriptors
2044 Mor30v	signal 30 / weighted by van der Waals volume	3D-MoRSE descriptors
2045 Mor31v	signal 31 / weighted by van der Waals volume	3D-MoRSE descriptors
2046 Mor32v	signal 32 / weighted by van der Waals volume	3D-MoRSE descriptors
2047 Mor01e	signal 01 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2048 Mor02e	signal 02 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2049 Mor03e	signal 03 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2050 Mor04e	signal 04 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2051 Mor05e	signal 05 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2052 Mor06e	signal 06 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2053 Mor07e	signal 07 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2054 Mor08e	signal 08 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2055 Mor09e	signal 09 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2056 Mor10e	signal 10 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2057 Mor11e	signal 11 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2058 Mor12e	signal 12 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2059 Mor13e	signal 13 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2060 Mor14e	signal 14 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2061 Mor15e	signal 15 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2062 Mor16e		
	signal 16 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2063 Mor17e	signal 17 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2064 Mor18e	signal 18 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2065 Mor19e	signal 19 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2066 Mor20e	signal 20 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2067 Mor21e	signal 21 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2068 Mor22e	signal 22 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2069 Mor23e	signal 23 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2070 Mor24e	signal 24 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2071 Mor25e	signal 25 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2072 Mor26e	signal 26 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2073 Mor27e	signal 27 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2074 Mor28e	signal 28 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2075 Mor29e	signal 29 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2076 Mor30e	signal 30 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2077 Mor31e	signal 31 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2078 Mor32e	signal 32 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
2079 Mor01p	signal 01 / weighted by polarizability	3D-MoRSE descriptors
2080 Mor02p	signal 02 / weighted by polarizability	3D-MoRSE descriptors
2081 Mor03p	signal 03 / weighted by polarizability	3D-MoRSE descriptors
2082 Mor04p	signal 04 / weighted by polarizability	3D-MoRSE descriptors
2083 Mor05p	signal 05 / weighted by polarizability	3D-MoRSE descriptors
2084 Mor06p	signal 06 / weighted by polarizability	3D-MoRSE descriptors
2085 Mor07p	signal 07 / weighted by polarizability	3D-MoRSE descriptors
2086 Mor08p	signal 08 / weighted by polarizability	3D-MoRSE descriptors
2087 Mor09p	signal 09 / weighted by polarizability	3D-MoRSE descriptors
2088 Mor10p	signal 10 / weighted by polarizability	3D-MoRSE descriptors
2089 Mor11p	signal 11 / weighted by polarizability	3D-MoRSE descriptors
2090 Mor12p	signal 12 / weighted by polarizability	3D-MoRSE descriptors
2091 Mor13p	signal 13 / weighted by polarizability	3D-MoRSE descriptors
2092 Mor14p	signal 14 / weighted by polarizability	3D-MoRSE descriptors
2093 Mor15p	signal 15 / weighted by polarizability	3D-MoRSE descriptors
2094 Mor16p	signal 16 / weighted by polarizability	3D-MoRSE descriptors
2095 Mor17p	signal 17 / weighted by polarizability	3D-MoRSE descriptors
2096 Mor18p	signal 18 / weighted by polarizability	3D-MoRSE descriptors
2097 Mor19p	signal 19 / weighted by polarizability	3D-MoRSE descriptors
2098 Mor20p	signal 20 / weighted by polarizability	3D-MoRSE descriptors
2099 Mor21p	signal 20 / weighted by polarizability signal 21 / weighted by polarizability	3D-MoRSE descriptors
2100 Mor22p	signal 22 / weighted by polarizability	3D-MoRSE descriptors
2101 Mor23p	signal 23 / weighted by polarizability	3D-Morse descriptors
2101 Mor23p 2102 Mor24p	signal 24 / weighted by polarizability	
		3D-MoRSE descriptors
2103 Mor25p	signal 25 / weighted by polarizability	3D-MoRSE descriptors
2104 Mor26p	signal 26 / weighted by polarizability	3D-MoRSE descriptors
2105 Mor27p	signal 27 / weighted by polarizability	3D-MoRSE descriptors
2106 Mor28p	signal 28 / weighted by polarizability	3D-MoRSE descriptors
2107 Mor29p	signal 29 / weighted by polarizability	3D-MoRSE descriptors
2108 Mor30p	signal 30 / weighted by polarizability	3D-MoRSE descriptors



2109 Mor31p	signal 31 / weighted by polarizability	3D-MoRSE descriptors
2110 Mor32p	signal 32 / weighted by polarizability	3D-MoRSE descriptors
2111 Mor01i	signal 01 / weighted by ionization potential	3D-MoRSE descriptors
2112 Mor02i	signal 02 / weighted by ionization potential	3D-MoRSE descriptors
2113 Mor03i	signal 03 / weighted by ionization potential	3D-MoRSE descriptors
2114 Mor04i	signal 04 / weighted by ionization potential	3D-MoRSE descriptors
2115 Mor05i	signal 05 / weighted by ionization potential	3D-MoRSE descriptors
2116 Mor06i	signal 06 / weighted by ionization potential	3D-MoRSE descriptors
2117 Mor07i	signal 07 / weighted by ionization potential	3D-MoRSE descriptors
2118 Mor08i	signal 08 / weighted by ionization potential	3D-MoRSE descriptors
2119 Mor09i	signal 09 / weighted by ionization potential	3D-MoRSE descriptors
2120 Mor10i	signal 10 / weighted by ionization potential	3D-MoRSE descriptors
2121 Mor11i		
	signal 11 / weighted by ionization potential	3D-MoRSE descriptors
2122 Mor12i	signal 12 / weighted by ionization potential	3D-MoRSE descriptors
2123 Mor13i	signal 13 / weighted by ionization potential	3D-MoRSE descriptors
2124 Mor14i	signal 14 / weighted by ionization potential	3D-MoRSE descriptors
2125 Mor15i	signal 15 / weighted by ionization potential	3D-MoRSE descriptors
2126 Mor16i	signal 16 / weighted by ionization potential	3D-MoRSE descriptors
2127 Mor17i	signal 17 / weighted by ionization potential	3D-MoRSE descriptors
2128 Mor18i	signal 18 / weighted by ionization potential	3D-MoRSE descriptors
2129 Mor19i	signal 19 / weighted by ionization potential	3D-MoRSE descriptors
2130 Mor20i	signal 20 / weighted by ionization potential	3D-MoRSE descriptors
2131 Mor21i	signal 21 / weighted by ionization potential	3D-MoRSE descriptors
2132 Mor22i	signal 22 / weighted by ionization potential	3D-MoRSE descriptors
2133 Mor23i	signal 23 / weighted by ionization potential	3D-MoRSE descriptors
2134 Mor24i	signal 24 / weighted by ionization potential	3D-MoRSE descriptors
2135 Mor25i	signal 25 / weighted by ionization potential	3D-MoRSE descriptors
2136 Mor26i	signal 26 / weighted by ionization potential	3D-MoRSE descriptors
2137 Mor27i	signal 27 / weighted by ionization potential	3D-MoRSE descriptors
2138 Mor28i	signal 28 / weighted by ionization potential	3D-MoRSE descriptors
2139 Mor29i	signal 29 / weighted by ionization potential signal 29 / weighted by ionization potential	3D-MoRSE descriptors
2140 Mor30i	signal 30 / weighted by ionization potential	3D-MoRSE descriptors
2141 Mor31i	signal 31 / weighted by ionization potential	3D-MoRSE descriptors
2142 Mor32i	signal 32 / weighted by ionization potential	3D-MoRSE descriptors
2143 Mor01s	signal 01 / weighted by I-state	3D-MoRSE descriptors
2144 Mor02s	signal 02 / weighted by I-state	3D-MoRSE descriptors
2145 Mor03s	signal 03 / weighted by I-state	3D-MoRSE descriptors
2146 Mor04s	signal 04 / weighted by I-state	3D-MoRSE descriptors
2147 Mor05s	signal 05 / weighted by I-state	3D-MoRSE descriptors
2148 Mor06s	signal 06 / weighted by I-state	3D-MoRSE descriptors
2149 Mor07s	signal 07 / weighted by I-state	3D-MoRSE descriptors
2150 Mor08s	signal 08 / weighted by I-state	3D-MoRSE descriptors
2151 Mor09s	signal 09 / weighted by I-state	3D-MoRSE descriptors
2152 Mor10s	signal 10 / weighted by I-state	3D-MoRSE descriptors
2153 Mor11s	signal 11 / weighted by I-state	3D-MoRSE descriptors
2154 Mor12s		
	signal 12 / weighted by I-state	3D-MoRSE descriptors
2155 Mor13s	signal 13 / weighted by I-state	3D-MoRSE descriptors
2156 Mor14s	signal 14 / weighted by I-state	3D-MoRSE descriptors
2157 Mor15s	signal 15 / weighted by I-state	3D-MoRSE descriptors
2158 Mor16s	signal 16 / weighted by I-state	3D-MoRSE descriptors
2159 Mor17s	signal 17 / weighted by I-state	3D-MoRSE descriptors
2160 Mor18s	signal 18 / weighted by I-state	3D-MoRSE descriptors
2161 Mor19s	signal 19 / weighted by I-state	3D-MoRSE descriptors
2162 Mor20s	signal 20 / weighted by I-state	3D-MoRSE descriptors
2163 Mor21s	signal 21 / weighted by I-state	3D-MoRSE descriptors
2164 Mor22s	signal 22 / weighted by I-state	3D-MoRSE descriptors
2165 Mor23s	signal 23 / weighted by I-state	3D-MoRSE descriptors
2166 Mor24s	signal 24 / weighted by I-state	3D-MoRSE descriptors
2167 Mor25s	signal 25 / weighted by I-state	3D-MoRSE descriptors
2168 Mor26s	signal 26 / weighted by I-state	3D-MoRSE descriptors
2169 Mor27s	signal 27 / weighted by I-state	3D-MoRSE descriptors
2170 Mor28s		3D-MoRSE descriptors
	signal 28 / weighted by I-state	
2171 Mor29s	signal 29 / weighted by I-state	3D-MoRSE descriptors
2172 Mor30s	signal 30 / weighted by I-state	3D-MoRSE descriptors
2173 Mor31s	signal 31 / weighted by I-state	3D-MoRSE descriptors
2174 Mor32s	signal 32 / weighted by I-state	3D-MoRSE descriptors
2175 L1u	1st component size directional WHIM index / unweighted	WHIM descriptors
2176 L2u	2nd component size directional WHIM index / unweighted	WHIM descriptors
2177 L3u	3rd component size directional WHIM index / unweighted	WHIM descriptors
2178 P1u	1st component shape directional WHIM index / unweighted	WHIM descriptors
2179 P2u	2nd component shape directional WHIM index / unweighted	WHIM descriptors
2180 G1u	1st component symmetry directional WHIM index / unweighted	WHIM descriptors
2181 G2u	2nd component symmetry directional WHIM index / unweighted	WHIM descriptors
2182 G3u	3rd component symmetry directional WHIM index / unweighted	WHIM descriptors
2183 E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
2184 E2u	2nd component accessibility directional WHIM index / unweighted	WHIM descriptors
2185 E3u	3rd component accessibility directional WHIM index / unweighted	WHIM descriptors
2186 L1m	1st component size directional WHIM index / weighted by mass	WHIM descriptors
2187 L2m	2nd component size directional WHIM index / weighted by mass	WHIM descriptors
2188 L3m	3rd component size directional WHIM index / weighted by mass	WHIM descriptors
2189 P1m	1st component shape directional WHIM index / weighted by mass	WHIM descriptors
2190 P2m	2nd component shape directional WHIM index / weighted by mass	WHIM descriptors
2191 G1m	1st component symmetry directional WHIM index / weighted by mass	WHIM descriptors
2192 G2m	2nd component symmetry directional WHIM index / weighted by mass	WHIM descriptors WHIM descriptors
2193 G3m	3rd component symmetry directional WHIM index / weighted by mass	WHIM descriptors
2194 E1m	1st component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2195 E2m	2nd component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2196 E3m	3rd component accessibility directional WHIM index / weighted by mass	WHIM descriptors
2197 L1v	1st component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2198 L2v	2nd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2199 L3v	3rd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2200 P1v		M/HIM descriptors
	1st component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2201 P2v	1st component shape directional WHIM index / weighted by van der Waals volume 2nd component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2202 G1v	2nd component shape directional WHIM index / weighted by van der Waals volume 1st component symmetry directional WHIM index / weighted by van der Waals volume	
	2nd component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2202 G1v	2nd component shape directional WHIM index / weighted by van der Waals volume 1st component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors WHIM descriptors



2205 E1v	1st component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2206 E2v	2nd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2207 E3v	3rd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors
2208 L1e	1st component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
		·
2209 L2e	2nd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2210 L3e	3rd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2211 P1e	1st component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2212 P2e	2nd component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2213 G1e	1st component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2214 G2e	2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2215 G3e	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2216 E1e	1st component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2217 E2e	2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2218 E3e	3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors
2219 L1p	1st component size directional WHIM index / weighted by polarizability	WHIM descriptors
2220 L2p	2nd component size directional WHIM index / weighted by polarizability	WHIM descriptors
2221 L3p	3rd component size directional WHIM index / weighted by polarizability	WHIM descriptors
		·
2222 P1p	1st component shape directional WHIM index / weighted by polarizability	WHIM descriptors
2223 P2p	2nd component shape directional WHIM index / weighted by polarizability	WHIM descriptors
2224 G1p	1st component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2225 G2p	2nd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2226 G3p	3rd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors
2227 E1p	1st component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2228 E2p	2nd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2229 E3p	3rd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors
2230 L1i	1st component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2231 L2i	2nd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2232 L3i	3rd component size directional WHIM index / weighted by ionization potential	WHIM descriptors
2233 P1i	1st component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
		·
2234 P2i	2nd component shape directional WHIM index / weighted by ionization potential	WHIM descriptors
2235 G1i	1st component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2236 G2i	2nd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2237 G3i	3rd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors
2238 E1i	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2239 E2i	2nd component accessibility directional WHIM index / weighted by ionization potential	
		WHIM descriptors
2240 E3i	3rd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
2241 L1s	1st component size directional WHIM index / weighted by I-state	WHIM descriptors
2242 L2s	2nd component size directional WHIM index / weighted by I-state	WHIM descriptors
2243 L3s	3rd component size directional WHIM index / weighted by I-state	WHIM descriptors
2244 P1s	1st component shape directional WHIM index / weighted by I-state	WHIM descriptors
2245 P2s	2nd component shape directional WHIM index / weighted by I-state	WHIM descriptors
2246 G1s	1st component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2247 G2s	2nd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2248 G3s	3rd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors
2249 E1s	1st component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2250 E2s	2nd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2251 E3s	3rd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors
2252 Tu	T total size index / unweighted	WHIM descriptors
2253 Tm	T total size index / weighted by mass	WHIM descriptors
2254 Tv	T total size index / weighted by van der Waals volume	WHIM descriptors
2255 Te	T total size index / weighted by Sanderson electronegativity	WHIM descriptors
2256 Tp	T total size index / weighted by polarizability	WHIM descriptors
2257 Ti	T total size index / weighted by ionization potential	WHIM descriptors
2258 Ts	T total size index / weighted by I-state	WHIM descriptors
2259 Au	A total size index / unweighted	WHIM descriptors
2260 Am	A total size index / weighted by mass	WHIM descriptors
2261 Av	A total size index / weighted by van der Waals volume	WHIM descriptors
2262 Ae	A total size index / weighted by Sanderson electronegativity	WHIM descriptors
2263 Ap	A total size index / weighted by polarizability	WHIM descriptors
2264 Ai	A total size index / weighted by ionization potential	WHIM descriptors
2265 As	A total size index / weighted by I-state	WHIM descriptors
2266 Gu	total symmetry index / unweighted	WHIM descriptors
2267 Gm	total symmetry index / unweighted by mass	WHIM descriptors
2268 Ku	K global shape index / unweighted	WHIM descriptors
2269 Km	K global shape index / weighted by mass	WHIM descriptors
2270 Kv	K global shape index / weighted by van der Waals volume	WHIM descriptors
2271 Ke	K global shape index / weighted by Sanderson electronegativity	WHIM descriptors
2272 Kp	K global shape index / weighted by polarizability	WHIM descriptors
2273 Ki	K global shape index / weighted by polarization potential	WHIM descriptors
		·
2274 Ks	K global shape index / weighted by I-state	WHIM descriptors
2275 Du	D total accessibility index / unweighted	WHIM descriptors
2276 Day	D total accessibility index / weighted by mass	WHIM descriptors
2276 Dm	D total accessibility index / weighted by mass	WHIM descriptors
2276 DIII 2277 Dv	D total accessibility index / weighted by mass D total accessibility index / weighted by van der Waals volume	
2277 Dv	D total accessibility index / weighted by van der Waals volume	WHIM descriptors
2277 Dv 2278 De	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity	WHIM descriptors
2277 Dv 2278 De 2279 Dp	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability	WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential	WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state	WHIM descriptors WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential	WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state	WHIM descriptors WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds 2282 Vu 2283 Vm	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state V total size index / unweighted V total size index / weighted by mass	WHIM descriptors WHIM descriptors WHIM descriptors WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds 2282 Vu 2283 Vm 2284 Vv	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state V total size index / unweighted V total size index / weighted by mass V total size index / weighted by was der Waals volume	WHIM descriptors WHIM descriptors WHIM descriptors WHIM descriptors WHIM descriptors WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds 2282 Vu 2283 Vm 2284 Vv 2285 Ve	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state V total size index / unweighted V total size index / weighted by mass V total size index / weighted by van der Waals volume V total size index / weighted by Sanderson electronegativity	WHIM descriptors
2277 Dv 2278 De 2279 Dp 2280 Di 2281 Ds 2282 Vu 2283 Vm 2284 Vv 2285 Ve 2286 Vp	D total accessibility index / weighted by van der Waals volume D total accessibility index / weighted by Sanderson electronegativity D total accessibility index / weighted by polarizability D total accessibility index / weighted by ionization potential D total accessibility index / weighted by I-state V total size index / unweighted V total size index / weighted by mass V total size index / weighted by van der Waals volume V total size index / weighted by Sanderson electronegativity V total size index / weighted by polarizability	WHIM descriptors
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2301 H8u
2302 HTu
2303 HATS0u
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2304 HATS1u
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2305 HATS2u
2306 HATS3u
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2307 HATS4u
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2308 HATS5u
2309 HATS6u
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2310 HATS7u
2311 HATS8u
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2312 HATSu
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2313 H0m
2314 H1m
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2315 H2m
2316 H3m
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2317 H4m
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2318 H5m
2319 H6m
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2320 H7m
2321 H8m
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2322 HTm
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2323 HATS0m
              HATS1m
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2325 HATS2m
2326 HATS3m
2327 HATS4m
2328 HATS5m
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2329 HATS6m
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2330 HATS7m
2331 HATS8m
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H autocorrelation of lag 0 / weighted by van der Waals volume
2332 HATSm
2333 H0v
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2334 H1v
2335 H2v
2336 H3v
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H autocorrelation of lag 5 / weighted by van der Waals volume
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2337 H4v
2338 H5v
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H autocorrelation of lag 7 / weighted by van der Waals volume
H autocorrelation of lag 8 / weighted by van der Waals volume
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2339 H6v
2340 H7v
2341 H8v
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2342 HTV
2343 HATS0v
                                                                        leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume leverage-weighted autocorrelation of lag 2 / weighted by van der Waals volume leverage-weighted autocorrelation of lag 3 / weighted by van der Waals volume leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume leverage-weighted autocorrelation of lag 5 / weighted by van der Waals volume
2344 HATS1v
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2345 HATS2v
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2346 HATS3v
2347 HATS4v
2348 HATS5v
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2349 HATS6v
2350 HATS7v
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2351 HATS8
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2352 HATSV
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2353 H0e
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2354 H1e
2355 H2e
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2356 H3e
2357 H4e
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2358 H5e
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2359 H6e
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2360 H7e
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2361 H8e
2362 HTe
2363 HATS0e
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2364 HATS1e
2365 HATS2e
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2366 HATS3e
2367 HATS4e
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2368 HATS5e
2369 HATS6e
2370 HATS7e
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2371 HATS8e
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2372 HATSe
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H autocorrelation of lag 1 / weighted by polarizability
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2373 H0p
2374 H1p
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2375 H2p
2376 H3p
2377 H4p
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2378 H5p
2379 H6p
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2380 H7p
2381 H8r
2382 HTp
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2383 HATS0p
2384 HATS1p
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2385 HATS2p
2386 HATS3p
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2387 HATS4p
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2388 HATS5p
2389 HATS6p
2390 HATS7p
2391 HATS8p
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2392 HATSp
                                                                          leverage-weighted total index / weighted by polarizability
                                                                        H autocorrelation of lag 0 / weighted by ionization potential H autocorrelation of lag 1 / weighted by ionization potential
2393 H0i
2394 H1i
                                                                                                                                                                                                                                                                                                                                                                  GETAWAY descriptors
                                                                        H autocorrelation of lag 2 / weighted by ionization potential H autocorrelation of lag 3 / weighted by ionization potential
                                                                                                                                                                                                                                                                                                                                                                 GETAWAY descriptors
GETAWAY descriptors
2395 H2i
2396 H3i
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H autocorrelation of lag 4 / weighted by ionization potential H autocorrelation of lag 5 / weighted by ionization potential
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2397 H4i
2398 H5i
2399 H6i
                                                          H autocorrelation of lag 6 / weighted by ionization potential H autocorrelation of lag 7 / weighted by ionization potential
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2400 H7i
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2401 H8i
                                                          H autocorrelation of lag 8 / weighted by ionization potential
2402 HT
                                                          H total index / weighted by ionization potential leverage-weighted autocorrelation of lag 0 / weighted by ionization potential
2403 HATS0i
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
2404 HATS1i
2405 HATS2i
                                                          leverage-weighted autocorrelation of lag 1 / weighted by ionization potential leverage-weighted autocorrelation of lag 2 / weighted by ionization potential
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
                                                          leverage-weighted autocorrelation of lag 2 / weighted by ionization potential leverage-weighted autocorrelation of lag 3 / weighted by ionization potential leverage-weighted autocorrelation of lag 4 / weighted by ionization potential leverage-weighted autocorrelation of lag 5 / weighted by ionization potential leverage-weighted autocorrelation of lag 6 / weighted by ionization potential leverage-weighted autocorrelation of lag 7 / weighted by ionization potential
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2406 HATS3i
2407 HATS4i
2408 HATS5i
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2409 HATS6i
2410 HATS7i
2411 HATS8i
2412 HATSi
                                                          leverage-weighted autocorrelation of lag 8 / weighted by ionization potential leverage-weighted total index / weighted by ionization potential
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2413 H0s
                                                          H autocorrelation of lag 0 / weighted by I-state
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
                                                          H autocorrelation of lag 1 / weighted by I-state H autocorrelation of lag 2 / weighted by I-state
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2414 H1s
2415 H2s
                                                          H autocorrelation of lag 3 / weighted by I-state
H autocorrelation of lag 4 / weighted by I-state
H autocorrelation of lag 5 / weighted by I-state
2416 H3s
2417 H4s
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                                                                                                                                                                                                                                                          GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
2418 H5s
                                                         H autocorrelation of lag 6 / weighted by I-state
H autocorrelation of lag 6 / weighted by I-state
H autocorrelation of lag 7 / weighted by I-state
H autocorrelation of lag 8 / weighted by I-state
H total index / weighted by I-state
leverage-weighted autocorrelation of lag 0 / weighted by I-state
leverage-weighted autocorrelation of lag 2 / weighted by I-state
leverage-weighted autocorrelation of lag 2 / weighted by I-state
leverage-weighted autocorrelation of lag 2 / weighted by I-state
leverage-weighted autocorrelation of lag 3 / weighted by I-state
2419 H6s
2420 H7s
2421 H8s
2422 HTs
2423 HATS0s
2424 HATS1s
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2425 HATS2s
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
                                                          leverage-weighted autocorrelation of lag 3 / weighted by I-state leverage-weighted autocorrelation of lag 4 / weighted by I-state
2426 HATS3s
2427 HATS4s
                                                          leverage-weighted autocorrelation of lag 5 / weighted by I-state leverage-weighted autocorrelation of lag 6 / weighted by I-state leverage-weighted autocorrelation of lag 7 / weighted by I-state leverage-weighted autocorrelation of lag 7 / weighted by I-state
2428 HATS5s
2429 HATS6s
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
2430 HATS7s
2431 HATS8s
                                                          leverage-weighted autocorrelation of lag 8 / weighted by I-state leverage-weighted total index / weighted by I-state
2432 HATSs
2433 RCON
2434 RARS
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          Randic-type R matrix connectivity
                                                          R matrix average row sum
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2435 REIG
                                                          first eigenvalue of the R matrix
                                                          R autocorrelation of lag 1 / unweighted R autocorrelation of lag 2 / unweighted
2436 R1u
2437 R2u
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
2438 R3u
2439 R4u
                                                          R autocorrelation of lag 3 / unweighted R autocorrelation of lag 4 / unweighted
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          R autocorrelation of lag 5 / unweighted R autocorrelation of lag 6 / unweighted R autocorrelation of lag 7 / unweighted
2440 R5u
2441 R6u
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
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GETAWAY descriptors
GETAWAY descriptors
2442 R7u
                                                          R autocorrelation of lag 8 / unweighted R total index / unweighted
2443 R8u
2444 RTu
2445 R1u+
2446 R2u+
                                                          R maximal autocorrelation of lag 1 / unweighted R maximal autocorrelation of lag 2 / unweighted
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2447
           R3u+
                                                          R maximal autocorrelation of lag 3 / unweighted
                                                          R maximal autocorrelation of lag 4 / unweighted R maximal autocorrelation of lag 5 / unweighted
2448 R4u+
2449 R5u+
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
                                                          R maximal autocorrelation of lag 6 / unweighted R maximal autocorrelation of lag 7 / unweighted
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2450 R6u+
2451 R7u+
                                                          R maximal autocorrelation of lag 8 / unweighted R maximal index / unweighted R autocorrelation of lag 1 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2452 R8u+
2453 RTu+
2454 R1m
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
2455 R2m
                                                          R autocorrelation of lag 2 / weighted by mass R autocorrelation of lag 3 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2456 R3m
                                                          R autocorrelation of lag 4 / weighted by mass R autocorrelation of lag 5 / weighted by mass R autocorrelation of lag 5 / weighted by mass R autocorrelation of lag 6 / weighted by mass R autocorrelation of lag 7 / weighted by mass R autocorrelation of lag 8 / weighted by mass R autocorrelation of lag 8 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2457 R4m
2458 R5m
2459 R6m
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2460 R7m
2461
           R8m
                                                          R total index / weighted by mass
R maximal autocorrelation of lag 1 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2462 RTm
2463 R1m+
                                                          R maximal autocorrelation of lag 2 / weighted by mass R maximal autocorrelation of lag 3 / weighted by mass R maximal autocorrelation of lag 4 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2464
           R2m+
2465 R3m+
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
2466 R4m+
2467 R5m+
                                                          R maximal autocorrelation of lag 5 / weighted by mass R maximal autocorrelation of lag 6 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2468 R6m+
                                                          R maximal autocorrelation of lag 7 / weighted by mass R maximal autocorrelation of lag 8 / weighted by mass
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2469 R7m+
2470 R8m+
2471 RTm+
                                                          R maximal index / weighted by mass
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          R autocorrelation of lag 1 / weighted by van der Waals volume R autocorrelation of lag 2 / weighted by van der Waals volume
2472 R1v
2473 R2v
2474 R3v
2475 R4v
                                                          R autocorrelation of lag 3 / weighted by van der Waals volume
R autocorrelation of lag 4 / weighted by van der Waals volume
R autocorrelation of lag 5 / weighted by van der Waals volume
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
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GETAWAY descriptors
GETAWAY descriptors
2476 R5v
                                                          R autocorrelation of lag 6 / weighted by van der Waals volume
R autocorrelation of lag 7 / weighted by van der Waals volume
2477 R6v
2478 R7v
2479 R8v
2480 RTv
                                                          R autocorrelation of lag 8 / weighted by van der Waals volume
R total index / weighted by van der Waals volume
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          R maximal autocorrelation of lag 1 / weighted by van der Waals volume R maximal autocorrelation of lag 2 / weighted by van der Waals volume R maximal autocorrelation of lag 3 / weighted by van der Waals volume
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
GETAWAY descriptors
2481 R1v+
2482 R2v+
2483 R3v+
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          R maximal autocorrelation of lag 4 / weighted by van der Waals volume R maximal autocorrelation of lag 5 / weighted by van der Waals volume
2484 R4v+
2485 R5v+
2486 R6v+
2487 R7v+
                                                          R maximal autocorrelation of lag 6 / weighted by van der Waals volume R maximal autocorrelation of lag 7 / weighted by van der Waals volume
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
2488 R8v+
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
                                                          R maximal autocorrelation of lag 8 / weighted by van der Waals volume
                                                          R maximal index / weighted by van der Waals volume R autocorrelation of lag 1 / weighted by Sanderson electronegativity
2489 RTv+
2490 R1e
                                                                                                                                                                                                                                                                                            GETAWAY descriptors
           R2e
                                                          R autocorrelation of lag 2 / weighted by Sanderson electronegativity R autocorrelation of lag 3 / weighted by Sanderson electronegativity
                                                                                                                                                                                                                                                                                           GETAWAY descriptors
GETAWAY descriptors
2491
2492 R3e
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2493 R4e	R autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors
2494 R5e	R autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2495 R6e	R autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2496 R7e	R autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2497 R8e	R autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2498 RTe	R total index / weighted by Sanderson electronegativity	GETAWAY descriptors
2499 R1e+	R maximal autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors
2500 R2e+	R maximal autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors
2501 R3e+ 2502 R4e+	R maximal autocorrelation of lag 3 / weighted by Sanderson electronegativity R maximal autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors GETAWAY descriptors
2502 R4e+ 2503 R5e+	R maximal autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors
2504 R6e+	R maximal autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors
2505 R7e+	R maximal autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors
2506 R8e+	R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors
2507 RTe+	R maximal index / weighted by Sanderson electronegativity	GETAWAY descriptors
2508 R1p	R autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors
2509 R2p	R autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2510 R3p	R autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors
2511 R4p	R autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors
2512 R5p	R autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2513 R6p	R autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2514 R7p	R autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2515 R8p	R autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2516 RTp	R total index / weighted by polarizability	GETAWAY descriptors
2517 R1p+	R maximal autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors
2518 R2p+ 2519 R3p+	R maximal autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors
2520 R4p+	R maximal autocorrelation of lag 3 / weighted by polarizability R maximal autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors GETAWAY descriptors
2521 R5p+	R maximal autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors
2522 R6p+	R maximal autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors
2523 R7p+	R maximal autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors
2524 R8p+	R maximal autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors
2525 RTp+	R maximal index / weighted by polarizability	GETAWAY descriptors
2526 R1i	R autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2527 R2i	R autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2528 R3i	R autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2529 R4i	R autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2530 R5i	R autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors
2531 R6i	R autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors
2532 R7i	R autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2533 R8i	R autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2534 RTi	R total index / weighted by ionization potential	GETAWAY descriptors
2535 R1i+	R maximal autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors
2536 R2i+	R maximal autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors
2537 R3i+	R maximal autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors
2538 R4i+ 2539 R5i+	R maximal autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors
2540 R6i+	R maximal autocorrelation of lag 5 / weighted by ionization potential R maximal autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors GETAWAY descriptors
2541 R7i+	R maximal autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors
2542 R8i+	R maximal autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors
2543 RTi+	R maximal index / weighted by ionization potential	GETAWAY descriptors
2544 R1s	R autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2545 R2s	R autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2546 R3s	R autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors
2547 R4s	R autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors
2548 R5s	R autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2549 R6s	R autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2550 R7s	R autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2551 R8s	R autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2552 RTs	R total index / weighted by I-state	GETAWAY descriptors
2553 R1s+	R maximal autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors
2554 R2s+	R maximal autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors
2555 R3s+ 2556 R4s+	R maximal autocorrelation of lag 3 / weighted by I-state R maximal autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors GETAWAY descriptors
2557 R5s+	R maximal autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors
2558 R6s+	R maximal autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors
2559 R7s+	R maximal autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors
2560 R8s+	R maximal autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors
2561 RTs+	R maximal index / weighted by I-state	GETAWAY descriptors
2562 DP01	molecular profile no. 1	Randic molecular profiles
2563 DP02	molecular profile no. 2	Randic molecular profiles
2564 DP03	molecular profile no. 3	Randic molecular profiles
2565 DP04	molecular profile no. 4	Randic molecular profiles
2566 DP05	molecular profile no. 5	Randic molecular profiles
2567 DP06	molecular profile no. 6	Randic molecular profiles
2568 DP07	molecular profile no. 7	Randic molecular profiles
2569 DP08	molecular profile no. 8	Randic molecular profiles
2570 DP09	molecular profile no. 9	Randic molecular profiles
2571 DP10	molecular profile no. 10	Randic molecular profiles
2572 DP11 2573 DP12	molecular profile no. 11	Randic molecular profiles
2573 DP12 2574 DP13	molecular profile no. 12 molecular profile no. 13	Randic molecular profiles Randic molecular profiles
2574 DP13 2575 DP14	molecular profile no. 13 molecular profile no. 14	Randic molecular profiles Randic molecular profiles
2576 DP14 2576 DP15	molecular profile no. 14 molecular profile no. 15	Randic molecular profiles Randic molecular profiles
2577 DP16	molecular profile no. 16	Randic molecular profiles
2578 DP17	molecular profile no. 17	Randic molecular profiles
2579 DP18	molecular profile no. 18	Randic molecular profiles
2580 DP19	molecular profile no. 19	Randic molecular profiles
2581 DP20	molecular profile no. 20	Randic molecular profiles
2582 SP01	shape profile no. 1	Randic molecular profiles
2583 SP02	shape profile no. 2	Randic molecular profiles
2584 SP03	shape profile no. 3	Randic molecular profiles
2585 SP04	shape profile no. 4	Randic molecular profiles
2586 SP05	shape profile no. 5	Randic molecular profiles
2587 SP06	shape profile no. 6	Randic molecular profiles
2588 SP07	shape profile no. 7	Randic molecular profiles



2589	SP08	shape profile no. 8	Randic molecular profiles
	SP09 SP10	shape profile no. 9	Randic molecular profiles
2591		shape profile no. 10 shape profile no. 11	Randic molecular profiles Randic molecular profiles
2593	SP12	shape profile no. 12	Randic molecular profiles
	SP13	shape profile no. 13	Randic molecular profiles
	SP14 SP15	shape profile no. 14 shape profile no. 15	Randic molecular profiles Randic molecular profiles
	SP16	shape profile no. 16	Randic molecular profiles
	SP17	shape profile no. 17	Randic molecular profiles
	SP18 SP19	shape profile no. 18 shape profile no. 19	Randic molecular profiles Randic molecular profiles
	SP20	shape profile no. 20	Randic molecular profiles
	SHP2	average shape profile index of order 2	Randic molecular profiles
2603		number of terminal primary C(sp3)	Functional group counts
2604 2605		number of total secondary C(sp3) number of total tertiary C(sp3)	Functional group counts Functional group counts
2606		number of total quaternary C(sp3)	Functional group counts
2607		number of ring secondary C(sp3)	Functional group counts
2608 2609		number of ring tertiary C(sp3) number of ring quaternary C(sp3)	Functional group counts Functional group counts
2610		number of aromatic C(sp2)	Functional group counts
	nCbH	number of unsubstituted benzene C(sp2)	Functional group counts
2612		number of substituted benzene C(sp2)	Functional group counts
	nCconj nR=Cp	number of non-aromatic conjugated C(sp2) number of terminal primary C(sp2)	Functional group counts Functional group counts
	nR=Cs	number of aliphatic secondary C(sp2)	Functional group counts
	nR=Ct	number of aliphatic tertiary C(sp2)	Functional group counts
	n=C= nR#CH/X	number of allenes groups number of terminal C(sp)	Functional group counts Functional group counts
	nR#C-	number of non-terminal C(sp)	Functional group counts
	nROCN	number of cyanates (aliphatic)	Functional group counts
	nArOCN	number of cyanates (aromatic)	Functional group counts
	nRNCO nArNCO	number of isocyanates (aliphatic) number of isocyanates (aromatic)	Functional group counts Functional group counts
	nRSCN	number of thiocyanates (aliphatic)	Functional group counts
	nArSCN	number of thiocyanates (aromatic)	Functional group counts
	nRNCS nArNCS	number of isothiocyanates (aliphatic) number of isothiocyanates (aromatic)	Functional group counts Functional group counts
	nRCOOH	number of carboxylic acids (aliphatic)	Functional group counts
	nArCOOH	number of carboxylic acids (aromatic)	Functional group counts
	nRCOOR nArCOOR	number of esters (aliphatic) number of esters (aromatic)	Functional group counts Functional group counts
	nRCONH2	number of esters (alornate) number of primary amides (aliphatic)	Functional group counts
	nArCONH2	number of primary amides (aromatic)	Functional group counts
	nRCONHR	number of secondary amides (aliphatic)	Functional group counts
	nArCONHR nRCONR2	number of secondary amides (aromatic) number of tertiary amides (aliphatic)	Functional group counts Functional group counts
	nArCONR2	number of tertiary amides (aromatic)	Functional group counts
	nROCON	number of (thio-) carbamates (aliphatic)	Functional group counts
	nArOCON nRCOX	number of (thio-) carbamates (aromatic) number of acyl halogenides (aliphatic)	Functional group counts Functional group counts
	nArCOX	number of acyl halogenides (aromatic)	Functional group counts
2642	nRCSOH	number of thioacids (aliphatic)	Functional group counts
	nArCSOH	number of thioacids (aromatic)	Functional group counts
	nRCSSH nArCSSH	number of dithioacids (aliphatic) number of dithioacids (aromatic)	Functional group counts Functional group counts
	nRCOSR	number of thioesters (aliphatic)	Functional group counts
	nArCOSR	number of thioesters (aromatic)	Functional group counts
	nRCSSR nArCSSR	number of dithioesters (aliphatic) number of dithioesters (aromatic)	Functional group counts Functional group counts
	nRCHO	number of aldehydes (aliphatic)	Functional group counts
	nArCHO	number of aldehydes (aromatic)	Functional group counts
	nRCO nArCO	number of ketones (aliphatic) number of ketones (aromatic)	Functional group counts Functional group counts
	nCONN	number of urea (-thio) derivatives	Functional group counts
2655	nC=O(O)2	number of carbonate (-thio) derivatives	Functional group counts
	nN=C-N<	number of amidine derivatives	Functional group counts
	nC(=N)N2 nRC=N	number of guanidine derivatives number of imines (aliphatic)	Functional group counts Functional group counts
2659	nArC=N	number of imines (aromatic)	Functional group counts
	nRCNO	number of oximes (aliphatic)	Functional group counts
	nArCNO nRNH2	number of oximes (aromatic) number of primary amines (aliphatic)	Functional group counts Functional group counts
	nArNH2	number of primary amines (aromatic)	Functional group counts
	nRNHR	number of secondary amines (aliphatic)	Functional group counts
	nArNHR nRNR2	number of secondary amines (aromatic) number of tertiary amines (aliphatic)	Functional group counts
	nArNR2	number of tertiary animes (ariphatic)	Functional group counts Functional group counts
2668	nN-N	number of N hydrazines	Functional group counts
	nN=N	number of N azo-derivatives	Functional group counts
	nRCN nArCN	number of nitriles (aliphatic) number of nitriles (aromatic)	Functional group counts Functional group counts
2672		number of intries (aromatic)	Functional group counts
2673	nNq	number of quaternary N	Functional group counts
	nRNHO nArNHO	number of hydroxylamines (aliphatic)	Functional group counts
	nRNNOx	number of hydroxylamines (aromatic) number of N-nitroso groups (aliphatic)	Functional group counts Functional group counts
2677	nArNNOx	number of N-nitroso groups (aromatic)	Functional group counts
	nRNO	number of nitroso groups (aliphatic)	Functional group counts
	nArNO nRNO2	number of nitroso groups (aromatic) number of nitro groups (aliphatic)	Functional group counts Functional group counts
	nArNO2	number of nitro groups (ampriatic)	Functional group counts
	nN(CO)2	number of imides (-thio)	Functional group counts
	nC=N-N< nROH	number of hydrazones number of hydroxyl groups	Functional group counts Functional group counts
2004			o.o.a. group counts



2659 ACPL				
2887 1094	2685 r	nArOH	number of aromatic hydroxyls	Functional group counts
288 offcold				
2868 InfOR				
260 IA/OR inambor of ellers issumated) Purchase you country Interest report in country Interest report				
2622 AND-CH2 Particles algorithms Part				
Page 2016-1972 Page				
2694 sti3CO			,, o , ,	
2616 66				
1987			number of thiols	
2688 ar New SSSR number of insulfaces Functional group counts 2701 a800H number of sulfaces Functional group counts 2701 a800H number of propagations Functional group counts 2702 a800H number of propagations Functional group counts 2703 a800H number of propagations Functional group counts 2703 a800H				
299 850				
Punctions group counts				· .
Processing Separation Proc				
2709 8-0300-H			· ·	
2704			,	
2706 nSO3				
2707 89C94				
2709 ePOSON number of pulphenshopsylhelian proposed in the process of pulphenshopsylhelian proposed in the process of pulphenshopsylhelian process of pulphens				
2709 in POS				
2711 nPFO number of phosphanes Fundoral group counts Fundoral group c				
2712 in Pri-O/Cide number of phosphorants (this) Functional group counts Functional grou				
2713 nFI-OREST			• •	
2714 nCH2RX		` '		
2719 RR-CRX				Functional group counts
2717 IRR-CHX				
2718 BR-CRX				.
2719 nRRCX				· .
Part			number of R#CX	Functional group counts
2722 R-CX2				
2723 ACRYS				
Purctional group counts				.
Purctional group counts				
Purctional group counts				
Purctional group counts Purctional group				
2731 Azetidines number of Thiranes Functional group counts F				
2723 Annotation number of Oxelanes Functional group counts				
2733 millorethanes				
Pyrolidines				
Process Proc				
2737 nth-Thiophenes number of Fertalydro-Iniophenes Functional group counts 2738 n Pyrroles number of Pyroles Functional group counts 2739 n Pyrazoles number of Pyrazoles Functional group counts 2740 n Imidazoles number of Furanes Functional group counts 2741 n Furanes number of Furanes Functional group counts 2743 n Holphenes number of Oxazoles Functional group counts 2743 n Holphenes number of Oxazoles Functional group counts 2744 n Hoszazoles number of Thiazoles Functional group counts 2746 n Institucions number of Thiazoles Functional group counts 2747 n friazoles number of Triazoles Functional group counts 2749 n Pyridazines number of Triazoles Functional group counts 2749 n Pyridines number of Triazoles Functional group counts 2740 n Pyridines number of Triazoles Functional group counts 2741 n Pyrazines punctional group counts 2751 n Pyrazines punctional group counts 2752 n 135-Triazines number of Triazoles Functional group counts <tr< td=""><td></td><td></td><td></td><td></td></tr<>				
2739 n Pyrrazoles number of Pyrazoles Functional group counts 2740 n Inidazoles number of Inidazoles Functional group counts 2741 n Furanes number of Inidazoles Functional group counts 2742 n Thiophenes number of Thiophenes Functional group counts 2743 n Oxazoles number of Thiophenes Functional group counts 2744 n Finazoles number of Isoxazoles Functional group counts 2744 n Finazoles number of Isoxazoles Functional group counts 2746 n Thiazoles number of Isoxazoles Functional group counts 2743 n Thiazoles number of Isoxazoles Functional group counts 2744 n Frydrazoles number of Isoxazoles Functional group counts 2743 n Triazoles number of Pyrididazoles Functional group counts 2744 n Prydrazoles number of Pyrididazoles Functional group counts 2750 n Pyrimidines number of Pyrimidizazoles Functional group counts 2751 n Pyrazoles number of Pyrimidizazoles Functional group counts 2752 n 135-Triazines number of 1-3-5-Triazines Functional group counts 2753 n 124-Tr				· .
2740 Infidazoles number of Inidazoles Functional group counts		nPyrroles	number of Pyrroles	Functional group counts
Purclinal group counts Purclinal group counts				
2742 Thiophenes number of Thiophenes Functional group counts				
2744 n Insoxazoles number of Isoxazoles Functional group counts 2745 n Thiazoles number of Thiazoles Functional group counts 2746 n Instituzoles number of Isothiazoles Functional group counts 2747 n Tritazoles number of Pyridines Functional group counts 2748 n Pyridazines number of Pyridines Functional group counts 2750 n Pyrinidines number of Pyrinidines Functional group counts 2751 n Pyrazines number of Pyrizines Functional group counts 2751 n Pyrazines number of 1-3-5-Triazines Functional group counts 2753 n 124-Triazines number of 1-24-Triazines Functional group counts 2754 n HDn number of 1-24-Triazines Functional group counts 2755 n HAcc number of acceptor atoms for H-bonds (N and O) Functional group counts 2755 n HAcc number of intramolecular H-bonds (N O,F) Functional group counts 2756 n HBonds number of intramolecular H-bonds (N O,F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2760 C-00				
2746 n Thiazoles number of Thiazoles Functional group counts 2747 n Triazoles number of triazoles Functional group counts 2748 n Pyridines number of Triazoles Functional group counts 2748 n Pyridianes number of Pyridianes Functional group counts 2749 n Pyrimidines number of Pyridianes Functional group counts 2750 n Pyrimidines number of Pyrizalnes Functional group counts 2752 n 135-Triazines number of Pyrazines Functional group counts 2753 n 124-Triazines number of 1-3-5-Triazines Functional group counts 2754 n HDon number of donor atoms for H-bonds (N and O) Functional group counts 2755 n HAcc number of donor atoms for H-bonds (N,O,F) Functional group counts 2756 n HBonds number of intramolecular H-bonds (With N,O,F) Functional group counts 2756 n HBonds number of intramolecular H-bonds (With N,O,F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2760 C-003 CH2R3 Atom-centred fragments 2761 C-005 </td <td></td> <td></td> <td></td> <td>.</td>				.
2748 nlsothiazoles number of Isothiazoles Functional group counts 2748 nPyridines number of Pyridianes Functional group counts 2748 nPyridazines number of Pyridianes Functional group counts 2750 nPyrinidines number of Pyridianes Functional group counts 2751 nPyrazines number of Pyrizines Functional group counts 2752 n135-Triazines number of Pyrizines Functional group counts 2753 n124-Triazines number of 1-24-Triazines Functional group counts 2753 n124-Triazines number of 1-24-Triazines Functional group counts 2754 nHDon number of acceptor atoms for H-bonds (N and O) Functional group counts 2755 nHAcc number of acceptor atoms for H-bonds (N,O,F) Functional group counts 2756 nHBonds number of acceptor atoms for H-bonds (With N,O,F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2760 C-003 CH83 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2XX				
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2749			number of Triazoles	Functional group counts
2750 R-yrimidines number of Pyrimidines number of Pyrazines number of 1-3-5-Triazines number of 1-2-4-Triazines number of donor atoms for H-bonds (N and O) number of donor atoms for H-bonds (N,O,F) number of acceptor atoms for H-bonds (N,O,F) Functional group counts Punctional group		,		
2751				
2753 nt24-Triazines number of 1-2-4-Triazines Functional group counts 2754 nHDon number of donor atoms for H-bonds (N.O.F) Functional group counts 2755 nHAcc number of acceptor atoms for H-bonds (N.O.F) Functional group counts 2756 nHBonds number of intramolecular H-bonds (with N.O.F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2759 C-003 CHR3 Atom-centred fragments 2760 C-004 CR4 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X2 Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2769 C-011 CR3X Atom-centred fragments 2769 C-012 CR2X2 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771		•	•	
2754 nHDon number of donor atoms for H-bonds (N and O) Functional group counts 2755 nHAcc number of acceptor atoms for H-bonds (N,O,F) Functional group counts 2756 nHBonds number of intramolecular H-bonds (with N,O,F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2760 C-003 CHR3 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2766 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2760 C-014 CX4 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-016 =CHR <td></td> <td></td> <td></td> <td>.</td>				.
2755 nHAcc number of acceptor atoms for H-bonds (N,O,F) Functional group counts 2756 nHBonds number of intramolecular H-bonds (with N,O,F) Functional group counts 2757 C-001 CH3R / CH4 Atom-centred fragments 2758 C-002 CH2R2 Atom-centred fragments 2760 C-003 CHR3 Atom-centred fragments 2760 C-004 CR4 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHRX2 Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 = CH2 Atom-centred fragments 2772 C-016 = CHR Atom-centred fragments<				
2756 nHBonds number of intramolecular H-bonds (with N,O,F) Functional group counts Atom-centred fragments Atom-centred fragmen				
2758 C-002 CH2R2 Atom-centred fragments 2759 C-003 CHR3 Atom-centred fragments 2760 C-004 CR4 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-014 CX4 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2775		nHBonds	number of intramolecular H-bonds (with N,O,F)	.
2759 C-003 CHR3 Atom-centred fragments 2760 C-004 CR4 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-014 CX4 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2776<				
2760 C-004 CR4 Atom-centred fragments 2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 = CH2 Atom-centred fragments 2772 C-016 = CHR Atom-centred fragments 2773 C-017 = CR2 Atom-centred fragments 2774 C-018 = CHX Atom-centred fragments 2775 C-019 = CRX Atom-centred fragments <td< td=""><td></td><td></td><td></td><td></td></td<>				
2761 C-005 CH3X Atom-centred fragments 2762 C-006 CH2RX Atom-centred fragments 2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 277				ū
2763 C-007 CH2X2 Atom-centred fragments 2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments <t< td=""><td></td><td></td><td>CH3X</td><td>Atom-centred fragments</td></t<>			CH3X	Atom-centred fragments
2764 C-008 CHR2X Atom-centred fragments 2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2765 C-009 CHRX2 Atom-centred fragments 2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2766 C-010 CHX3 Atom-centred fragments 2767 C-011 CR3X Atom-centred fragments 2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 = CH2 Atom-centred fragments 2772 C-016 = CHR Atom-centred fragments 2773 C-017 = CR2 Atom-centred fragments 2774 C-018 = CHX Atom-centred fragments 2775 C-019 = CRX Atom-centred fragments 2776 C-020 = CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2768 C-012 CR2X2 Atom-centred fragments 2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 = CH2 Atom-centred fragments 2772 C-016 = CHR Atom-centred fragments 2773 C-017 = CR2 Atom-centred fragments 2774 C-018 = CHX Atom-centred fragments 2775 C-019 = CRX Atom-centred fragments 2776 C-020 = CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments			CHX3	
2769 C-013 CRX3 Atom-centred fragments 2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2770 C-014 CX4 Atom-centred fragments 2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2771 C-015 =CH2 Atom-centred fragments 2772 C-016 =CHR Atom-centred fragments 2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2773 C-017 =CR2 Atom-centred fragments 2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments	2771 (C-015	=CH2	Atom-centred fragments
2774 C-018 =CHX Atom-centred fragments 2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2775 C-019 =CRX Atom-centred fragments 2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2776 C-020 =CX2 Atom-centred fragments 2777 C-021 #CH Atom-centred fragments 2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments				
2778 C-022 #CR / R=C=R Atom-centred fragments 2779 C-023 #CX Atom-centred fragments	2776 (C-020	=CX2	Atom-centred fragments
2779 C-023 #CX Atom-centred fragments				
· · · · · · · · · · · · · · · · · · ·				
				-

2781 C-025		
	5 RCRR	Atom-centred fragments
2782 C-026		Atom-centred fragments
2783 C-027		Atom-centred fragments
2784 C-028		Atom-centred fragments
2785 C-029		Atom-centred fragments
2786 C-030		Atom-centred fragments
2787 C-031		Atom-centred fragments
2788 C-032		Atom-centred fragments
2789 C-033		Atom-centred fragments
2790 C-034		Atom-centred fragments
2791 C-035		Atom-centred fragments
2792 C-036		Atom-centred fragments
2793 C-037		Atom-centred fragments
2794 C-038		Atom-centred fragments
2795 C-039		Atom-centred fragments
2796 C-040		Atom-centred fragments
2797 C-041		Atom-centred fragments
2798 C-042	· ·	Atom-centred fragments
2799 C-043		Atom-centred fragments
2800 C-044		Atom-centred fragments
2801 H-046		Atom-centred fragments
2802 H-047		Atom-centred fragments
2803 H-048	(1, (1,	Atom-centred fragments
2804 H-049		Atom-centred fragments
2805 H-050		Atom-centred fragments
2806 H-051		Atom-centred fragments
2807 H-052		Atom-centred fragments
2808 H-053		Atom-centred fragments
2809 H-054		Atom-centred fragments
2810 H-055	5 H attached to C0(sp3) with 4X attached to next C	Atom-centred fragments
2811 O-056		Atom-centred fragments
2812 O-057	7 phenol / enol / carboxyl OH	Atom-centred fragments
2813 O-058		Atom-centred fragments
2814 O-059	9 Al-O-Al	Atom-centred fragments
2815 O-060	0 Al-O-Ar / Ar-O-Ar / ROR / R-O-C=X	Atom-centred fragments
2816 O-061	·1 O	Atom-centred fragments
2817 O-062	O- (negatively charged)	Atom-centred fragments
2818 O-063	3 R-O-O-R	Atom-centred fragments
2819 Se-06-	64 Any-Se-Any	Atom-centred fragments
2820 Se-06	65 #NOME?	Atom-centred fragments
2821 N-066	6 Al-NH2	Atom-centred fragments
2822 N-067	7 Al2-NH	Atom-centred fragments
2823 N-068	8 Al3-N	Atom-centred fragments
2824 N-069	9 Ar-NH2 / X-NH2	Atom-centred fragments
2825 N-070	0 Ar-NH-Al	Atom-centred fragments
2826 N-071	1 Ar-NAI2	Atom-centred fragments
2827 N-072	2 RCO-NN-X=X	Atom-centred fragments
2828 N-073	3 Ar2NH / Ar3N / Ar2N-Al / RNR	Atom-centred fragments
2829 N-074	4 R#N / R=N-	Atom-centred fragments
2830 N-075	5 RNR / RNX	Atom-centred fragments
2831 N-076	6 Ar-NO2 / RN(R)O / RO-NO	Atom-centred fragments
2832 N-077	7 Al-NO2	
	741102	Atom-centred fragments
2833 N-078		
2833 N-078 2834 N-079	8 Ar-N=X / X-N=X	Atom-centred fragments
	8 Ar-N=X / X-N=X 9 N+ (positively charged)	Atom-centred fragments Atom-centred fragments
2834 N-079	8 Ar-N=X / X-N=X 9 N+ (positively charged) 1 F attached to C1(sp3)	Atom-centred fragments Atom-centred fragments Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083	8	Atom-centred fragments Atom-centred fragments Atom-centred fragments Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086 2841 CI-087	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-089 2844 Cl-090	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086 2841 CI-087 2842 CI-088 2844 CI-096 2845 Br-091	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-088 2844 Cl-096 2845 Br-091 2846 Br-092	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2840 Cl-086 2841 Cl-086 2842 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2842 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086 2841 CI-087 2842 CI-088 2844 CI-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-095	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-089 2844 Cl-090 2845 Br-091 2846 Br-092 2848 Br-092 2849 Br-092	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086 2841 CI-087 2842 CI-088 2843 CI-086 2844 CI-090 2845 Br-092 2847 Br-093 2848 Br-092 2849 Br-092 2851 I-097	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-098 2845 Br-091 2846 Br-092 2847 Br-092 2848 Br-092 2849 Br-096 2850 l-096 2851 l-097	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 CI-086 2841 CI-087 2842 CI-088 2844 CI-097 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-095 2850 I-096 2851 I-097 2852 I-098	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-092 2851 l-097 2852 l-098 2853 l-099	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-082 2844 Br-092 2845 Br-091 2846 Br-092 2849 Br-092 2849 Br-092 2850 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2848 Br-092 2849 Br-092 2851 l-096 2851 l-097 2852 l-098 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-086 2842 Cl-086 2843 Gl-086 2844 Br-097 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-092 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C3(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C3(sp3) C1 attached to C1(sp2) C1 attached to C3(sp3) C2 attached to C3(sp3) C3 C3 C4 C5	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-088 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-096 2851 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 F-101 2856 F-101 2858 I-104 2859 S-106	8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-080 2844 R-090 2845 Br-091 2846 Br-092 2847 Br-092 2848 Br-092 2849 Br-092 2851 l-097 2852 l-098 2853 l-104 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C1(sp2) C1 attached to C1(sp2) C2 attached to C1(sp2) C3 Br attached to C1(sp3) Br attached to C1(sp3) Br attached to C2(sp3)-C4(sp2)/C1(sp)/C4(sp3)/X Br attached to C3(sp3) I attached to C3(sp3)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-092 2847 Br-093 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X D1 Br attached to C1(sp2) D1 C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X D2 Br attached to C2(sp3) D3 Br attached to C2(sp3) D4 Br attached to C2(sp2) D5 Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X D6 D7 D8	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-088 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2848 Br-092 2850 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C1(sp2) C1 attached to C1(sp2) C1 attached to C1(sp2) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X F attached to C1(sp2) C2 Br attached to C2(sp3) Br attached to C2(sp3) Br attached to C2(sp3) Br attached to C2(sp3) Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X I attached to C1(sp3) I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X I attached to C2(sp3) I attached to C3(sp3)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-092 2845 Br-091 2846 Br-092 2851 I-097 2851 I-097 2852 I-098 2853 I-109 2855 F-101 2856 Cl-102 2857 Br-103 2858 I-104 2859 S-106 2861 S-108 2862 S-109 2863 S-110	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C1(sp2) C1 attached to C1(sp2) C1 attached to C1(sp2) C2 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C3 Br attached to C1(sp3) C3 Br attached to C2(sp3) C4 Br attached to C2(sp3) C5 Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C6 Br attached to C2(sp2) C6 Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C7 Br attached to C2(sp2) C8 Br attached to C2(sp2) C1 Br attached to C2(sp2) C2 Br attached to C3(sp3) C3 Br attached to C3(sp3) C4 Br attached to C3(sp3) C5 Br attached to C3(sp3) C6 Br attached to C3(sp3) C7 Br attached to C3(sp3) C8 Br attached to C3(sp3) C9 B	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-097 2845 Br-097 2846 Br-092 2847 Br-093 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2857 Br-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 S-109	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C1(sp2) C1 attached to C1(sp2) C2 attached to C1(sp2) C3 Br attached to C1(sp3) C3 Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C3 Br attached to C3(sp3) C3 Br attached to C3(sp3) C4 Br attached to C3(sp3) C5 Br attached to C3(sp3) C6 Br attached to C3(sp3) C7 Br attached to C3(sp3) C8 Br attached to C3(sp3) C9 Br attached to C3(sp3) C1 Br attached to C3(sp3) C2 Br attached to C3(sp3) C3 Br attached to C3(sp3) C4 Br attached to C3(sp3) C5 Br attached to C3(sp3) C6 Br attached to C3(sp3) C7 Br attached to C3(sp3) C8 Br attached to C3(sp3) C9 Br attached to C3(sp3)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-093 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2865 B-112 2866 P-115	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C1(sp3) C1 attached to C1(sp2) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Br attached to C2(sp3) Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X I attached to C2(sp3) I attached to C3(sp3) I a	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-092 2848 Br-092 2849 Br-095 2851 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2851 S-108 2853 S-109 2854 S-109 2853 S-106 2857 Br-103 2858 S-106 2859 S-107 2851 S-108 2852 S-109	Ar-N=X / X-N=X N + (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Cl attached to C1(sp3) Cl attached to C2(sp3) Cl attached to C3(sp3) Cl attached to C3(sp3) Cl attached to C1(sp2) Cl attached to C1(sp2) Cl attached to C1(sp2) Cl attached to C1(sp3) Br attached to C1(sp3) Br attached to C1(sp3) Br attached to C1(sp3) Br attached to C2(sp3) Br attached to C3(sp3) Br attached to C3(sp3) Ar Br attached to C3(sp3) Br at	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2845 Br-097 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-092 2849 Br-092 2851 l-097 2852 l-098 2853 l-104 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2866 B-112 2866 P-115 2867 P-116	Ar-N=X / X-N=X N+ (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C1(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C1(sp3) C2 attached to C1(sp3) C3 c1 attached to C1(sp2) C1 attached to C1(sp2) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Br attached to C1(sp3) Br attached to C2(sp3) Br attached to C3(sp3) I attached to C3(sp3)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-086 2843 Cl-086 2844 Cl-090 2845 Br-091 2846 Br-092 2847 Br-092 2847 Br-093 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2865 B-112 2866 P-115 2867 P-116	Ar-N=X / X-N=X N + (positively charged) F attached to C1(sp3) F attached to C2(sp3) F attached to C3(sp3) F attached to C3(sp3) F attached to C1(sp2) F attached to C1(sp2) F attached to C1(sp3) Cl attached to C1(sp3) Cl attached to C2(sp3) Cl attached to C3(sp3) Cl attached to C3(sp3) Cl attached to C1(sp2) Cl attached to C1(sp2) Cl attached to C1(sp2) Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Br attached to C1(sp3) Br attached to C3(sp3) Br attached to C3(sp3) Br attached to C3(sp3) Br attached to C2(sp3) Br attached to C2(sp3) Br attached to C2(sp3) Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X I attached to C3(sp3) I at	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Er-094 2849 Br-092 2848 Br-092 2849 Br-093 2848 Br-094 2849 Br-096 2851 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 El-102 2857 Br-103 2858 l-104 2859 S-106 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2866 B-115 2866 P-115 2867 P-116 2868 P-117 2869 P-118	Ar-N=X / X-N=X N+ (positively charged)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-092 2845 Br-091 2846 Br-092 2847 Br-092 2848 Br-092 2851 l-097 2852 l-098 2853 l-109 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2865 B-1112 2866 P-115 2867 P-116 2868 P-117 2869 P-118 2870 P-119	Ar-N=X / X-N=X N+ (positively charged)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-097 2845 Br-097 2846 Br-092 2847 Br-093 2850 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2857 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-110 2864 S-111 2866 B-115 2867 P-116 2868 P-117 2869 P-118 2870 P-118 2870 P-118 2871 P-120 2872 SSCH:	Ar-N=X / X-N=X N+ (positively charged)	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-088 2844 Cl-090 2845 Br-094 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-096 2851 l-096 2851 l-097 2852 l-098 2853 l-099 2854 l-100 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2866 P-115 2867 P-116 2868 P-117 2869 P-117 2869 P-118 2870 P-119 2871 P-120 2872 SSCH:	Ar-N=X / X.N=X N+ (positively charged) Fattached to C2(sp3) Fattached to C2(sp3) Fattached to C2(sp3) Fattached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Clattached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Clattached to C2(sp3) Clattached to C3(sp3) Clattached to C3(sp3) Clattached to C3(sp3) Clattached to C3(sp3) Clattached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Tattached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X Tattached to C2(sp3) Tattached to C3(sp3) Tattache	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Gl-089 2844 Br-092 2846 Br-092 2847 Br-093 2848 Br-094 2850 l-096 2851 l-097 2852 l-098 2853 l-109 2855 F-101 2856 Cl-102 2857 Br-103 2858 l-104 2859 S-106 2860 S-107 2861 S-108 2862 S-109 2863 S-111 2866 B-115 2867 P-116 2868 P-117 2869 P-118 2870 P-118 2871 P-120 2872 SSCH- 2873 SdCH- 2873 SdCH- 2874 SSSCH-	Ar-N=X / X.N=X N+ (positively charged) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X B1 C1 attached to C1(sp2) C2 C1 attached to C2(sp3) C3 C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X B2 C3	Atom-centred fragments
2834 N-079 2835 F-081 2836 F-082 2837 F-083 2838 F-084 2839 F-085 2840 Cl-086 2841 Cl-086 2841 Cl-087 2842 Cl-088 2843 Cl-088 2844 Cl-090 2845 Br-094 2846 Br-092 2847 Br-093 2848 Br-094 2849 Br-094 2851 l-096 2851 l-097 2852 l-098 2851 l-109 2853 l-099 2854 l-100 2855 F-101 2856 F-101 2858 l-104 2859 S-106 2861 S-108 2862 S-109 2863 S-110 2864 Si-111 2866 P-115 2867 P-116 2868 P-117 2869 P-117 2869 P-118 2870 P-119 2871 P-120 2872 SSCH: 2873 SdCH:	A-N=X / X.N=X N+ (positively charged) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp3) F attached to C2(sp2) F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X C1 attached to C2(sp3) C1 attached to C2(sp3) C1 attached to C3(sp3) C1 attached to C3(sp3) C1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X B1 attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X B2 B3 attached to C2(sp3) B3 B4 attached to C3(sp3) B5 B5 B7 attached to C3(sp3) B7 attached to C3(sp3) B8 attached to C3(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X B8 attached to C3(sp3) B9 attached t	Atom-centred fragments

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

Atom-type E-state indices Atom-type E-state indices
Atom-type E-state indices Atom-type E-state indices

Number of atoms of type sssN Number of atoms of type dsN 2973 NsssN 2974 NdsN 2975 NaaN Number of atoms of type aaN 2976 NtN Number of atoms of type tN 2977 NsNH3+ Number of atoms of type sNH3+ 2978 NssNH2+ Number of atoms of type ssNH2+ 2979 NdNH2+ Number of atoms of type dNH2+ Number of atoms of type sssNH+ Number of atoms of type ssssN+ 2980 NsssNH+ NssssN+ 2981 2982 NddsN Number of atoms of type ddsN 2983 NaasN Number of atoms of type aasN Number of atoms of type aaNH 2984 NaaNH Number of atoms of type sOH Number of atoms of type dO 2985 NsOH 2986 NdO 2987 NssO Number of atoms of type ssO 2988 NaaC Number of atoms of type aaC 2989 NsPH2 Number of atoms of type sPH2 Number of atoms of type ssPH Number of atoms of type sssP 2990 NssPH 2991 NsssF 2992 NdsssP Number of atoms of type dsssP 2993 NddsP Number of atoms of type ddsF 2994 NsssssP Number of atoms of type sssssP 2995 NsSH Number of atoms of type sSH Number of atoms of type dS 2996 NdS 2997 NssS Number of atoms of type ssS 2998 NaaS Number of atoms of type aaS 2999 NdssS 3000 NddssS Number of atoms of type dssS Number of atoms of type ddssS Number of atoms of type ssssssS 3001 NsssssS 3002 NsF Number of atoms of type sF 3003 NsCI Number of atoms of type sCI 3004 NsBr 3005 NsI Number of atoms of type sBr Number of atoms of type sl 3006 NsLi Number of atoms of type sLi 3007 NssBe Number of atoms of type ssBe Number of atoms of type ssssBe 3008 NssssBe-Number of atoms of type sBH2 Number of atoms of type ssBH 3009 NsBH2 3010 NssBH 3011 NsssB Number of atoms of type sssB 3012 NssssB Number of atoms of type ssssB-3013 NsGeH3 Number of atoms of type sGeH3 Number of atoms of type ssGeH2 Number of atoms of type sssGeH 3014 NssGeH2 3015 NsssGeH 3016 NssssGe Number of atoms of type ssssGe 3017 NsAsH2 Number of atoms of type sAsH2 3018 NssAsH Number of atoms of type ssAsH 3019 NsssAs Number of atoms of type sssAs 3020 NsssssAs Number of atoms of type sssssAs 3021 NdsssAs Number of atoms of type dsssAs Number of atoms of type ddsAs 3022 NddsAs 3023 NsSeH Number of atoms of type sSeH 3024 NdSe Number of atoms of type dSe 3025 NssSe Number of atoms of type ssSe Number of atoms of type aaSe Number of atoms of type dssSe 3026 NaaSe 3027 NdssSe 3028 NsssssSe Number of atoms of type ssssssSe 3029 NddssSe Number of atoms of type ddssSe 3030 NsSnH3 Number of atoms of type sSnH3 3031 NssSnH2 Number of atoms of type ssSnH2 Number of atoms of type sssSnH NsssSnH 3032 3033 NssssSn Number of atoms of type ssssSn 3034 NsPbH3 Number of atoms of type sPbH3 3035 NssPbH2 Number of atoms of type ssPbH2 3036 NsssPbH Number of atoms of type sssPbH 3037 NssssPb Number of atoms of type ssssPb 3038 NsSiH3 Number of atoms of type sSiH3 3039 NssSiH2 Number of atoms of type ssSiH2 3040 NsssSiH Number of atoms of type sssSiH 3041 NssssSi Number of atoms of type ssssSi CATS2D Donor-Donor at lag 00 3042 CATS2D_00_DD 3043 CATS2D_01_DD 3044 CATS2D 02 DD CATS2D Donor-Donor at lag 01 CATS2D Donor-Donor at lag 02 CATS2D Donor-Donor at lag 03 CATS2D Donor-Donor at lag 04 3045 CATS2D_03_DD 3046 CATS2D 04 DD CATS2D_05_DD CATS2D Donor-Donor at lag 05 3048 CATS2D_06_DD 3049 CATS2D_07_DD CATS2D Donor-Donor at lag 06 CATS2D Donor-Donor at lag 07 3050 CATS2D_08_DD 3051 CATS2D_09_DD CATS2D Donor-Donor at lag 08 CATS2D Donor-Donor at lag 09 3052 CATS2D_00_DA CATS2D Donor-Acceptor at lag 00 3053 CATS2D 01 DA CATS2D Donor-Acceptor at lag 01 CATS2D_02_DA CATS2D Donor-Acceptor at lag 02 3055 CATS2D_03_DA 3056 CATS2D_04_DA CATS2D Donor-Acceptor at lag 03 CATS2D Donor-Acceptor at lag 04 3057 CATS2D_05_DA CATS2D Donor-Acceptor at lag 05 3058 CATS2D 06 DA CATS2D Donor-Acceptor at lag 06 CATS2D_07_DA CATS2D Donor-Acceptor at lag 07 3060 CATS2D_08_DA 3061 CATS2D_09_DA CATS2D Donor-Acceptor at lag 08 CATS2D Donor-Acceptor at lag 09 3062 CATS2D_00_DP 3063 CATS2D_01_DP CATS2D Donor-Positive at lag 00 CATS2D Donor-Positive at lag 01 CATS2D Donor-Positive at lag 02 CATS2D Donor-Positive at lag 03 CATS2D_02_DP 3065 CATS2D_03_DP 3066 CATS2D_04_DP CATS2D Donor-Positive at lag 04 3067 CATS2D_05_DP 3068 CATS2D_06_DP CATS2D Donor-Positive at lag 05 CATS2D Donor-Positive at lag 06

Atom-type E-state indices Atom-type E-state indices
Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices Atom-type E-state indices CATS 2D CATS 2D CATS 2D

CATS 2D CATS 2D

3069 CATS2D_07_DP	CATS2D Donor-Positive at lag 07	CATS 2D
3070 CATS2D_08_DP	CATS2D Donor-Positive at lag 08	CATS 2D
3071 CATS2D_09_DP	CATS2D Donor-Positive at lag 09	CATS 2D
3072 CATS2D_00_DN	CATS2D Donor-Negative at lag 00	CATS 2D
3073 CATS2D_01_DN	CATS2D Donor-Negative at lag 01	CATS 2D
3074 CATS2D_02_DN	CATS2D Donor-Negative at lag 02	CATS 2D
3075 CATS2D_03_DN	CATS2D Donor-Negative at lag 03	CATS 2D
3076 CATS2D_04_DN	CATS2D Donor-Negative at lag 04	CATS 2D
3077 CATS2D_05_DN	CATS2D Donor-Negative at lag 05	CATS 2D
3078 CATS2D_06_DN	CATS2D Donor-Negative at lag 06	CATS 2D
3079 CATS2D_07_DN	CATS2D Donor-Negative at lag 07	CATS 2D
3080 CATS2D_08_DN	CATS2D Donor-Negative at lag 08	CATS 2D
3081 CATS2D_09_DN	CATS2D Donor-Negative at lag 09	CATS 2D
3082 CATS2D_00_DL	CATS2D Donor-Lipophilic at lag 00	CATS 2D
3083 CATS2D_01_DL	CATS2D Donor-Lipophilic at lag 01	CATS 2D
3084 CATS2D_02_DL	CATS2D Donor-Lipophilic at lag 02	CATS 2D
3085 CATS2D_03_DL 3086 CATS2D 04 DL	CATS2D Donor-Lipophilic at lag 03	CATS 2D
	CATS2D Donor-Lipophilic at lag 04	CATS 2D
3087 CATS2D_05_DL	CATS2D Donor-Lipophilic at lag 05	CATS 2D
3088 CATS2D_06_DL	CATS2D Donor-Lipophilic at lag 06	CATS 2D
3089 CATS2D_07_DL	CATS2D Donor-Lipophilic at lag 07	CATS 2D
3090 CATS2D_08_DL	CATS2D Donor-Lipophilic at lag 08	CATS 2D
3091 CATS2D_09_DL	CATS2D Donor-Lipophilic at lag 09	CATS 2D
3092 CATS2D_00_AA	CATS2D Acceptor-Acceptor at lag 00	CATS 2D
3093 CATS2D_01_AA 3094 CATS2D_02_AA	CATS2D Acceptor-Acceptor at lag 01	CATS 2D
	CATS2D Acceptor-Acceptor at lag 02	CATS 2D
3095 CATS2D_03_AA 3096 CATS2D 04 AA	CATS2D Acceptor Acceptor at lag 03	CATS 2D
3097 CATS2D_04_AA	CATS2D Acceptor Acceptor at lag 04	CATS 2D CATS 2D
3098 CATS2D_05_AA	CATS2D Acceptor Acceptor at lag 05	CATS 2D
3099 CATS2D_00_AA	CATS2D Acceptor-Acceptor at lag 06 CATS2D Acceptor-Acceptor at lag 07	CATS 2D
3100 CATS2D_07_AA		
3101 CATS2D_08_AA 3101 CATS2D_09_AA	CATS2D Acceptor-Acceptor at lag 08 CATS2D Acceptor-Acceptor at lag 09	CATS 2D CATS 2D
	CATS2D Acceptor-Acceptor at lag 09 CATS2D Acceptor-Positive at lag 00	CATS 2D CATS 2D
3102 CATS2D_00_AP 3103 CATS2D 01 AP	CATS2D Acceptor-Positive at lag 00 CATS2D Acceptor-Positive at lag 01	
3104 CATS2D_01_AP	CATS2D Acceptor-Positive at lag 01 CATS2D Acceptor-Positive at lag 02	CATS 2D CATS 2D
3105 CATS2D_02_AP	CATS2D Acceptor-Positive at lag 02 CATS2D Acceptor-Positive at lag 03	CATS 2D CATS 2D
3106 CATS2D_03_AP	CATS2D Acceptor-Positive at lag 03	CATS 2D
3107 CATS2D_04_AP	CATS2D Acceptor-Positive at lag 04	CATS 2D
3108 CATS2D_05_AF	CATS2D Acceptor-Positive at lag 05	CATS 2D
3109 CATS2D_00_AP	CATS2D Acceptor-Positive at lag 00	CATS 2D
3110 CATS2D 08 AP	CATS2D Acceptor-Positive at lag 08	CATS 2D
3111 CATS2D_00_AP	CATS2D Acceptor-Positive at lag 09	CATS 2D
3112 CATS2D_00_AN	CATS2D Acceptor-Negative at lag 00	CATS 2D
3113 CATS2D_01_AN	CATS2D Acceptor-Negative at lag 01	CATS 2D
3114 CATS2D_02_AN	CATS2D Acceptor-Negative at lag 01	CATS 2D
3115 CATS2D 03 AN	CATS2D Acceptor-Negative at lag 03	CATS 2D
3116 CATS2D 04 AN	CATS2D Acceptor-Negative at lag 04	CATS 2D
3117 CATS2D 05 AN	CATS2D Acceptor-Negative at lag 05	CATS 2D
3118 CATS2D_06_AN	CATS2D Acceptor-Negative at lag 06	CATS 2D
3119 CATS2D_07_AN	CATS2D Acceptor-Negative at lag 07	CATS 2D
3120 CATS2D_08_AN	CATS2D Acceptor-Negative at lag 08	CATS 2D
3121 CATS2D_09_AN	CATS2D Acceptor-Negative at lag 09	CATS 2D
3122 CATS2D 00 AL	CATS2D Acceptor-Lipophilic at lag 00	CATS 2D
3123 CATS2D 01 AL	CATS2D Acceptor-Lipophilic at lag 01	CATS 2D
3124 CATS2D 02 AL	CATS2D Acceptor-Lipophilic at lag 02	CATS 2D
3125 CATS2D_03_AL	CATS2D Acceptor-Lipophilic at lag 03	CATS 2D
3126 CATS2D_04_AL	CATS2D Acceptor-Lipophilic at lag 04	CATS 2D
3127 CATS2D 05 AL	CATS2D Acceptor-Lipophilic at lag 05	CATS 2D
3128 CATS2D 06 AL	CATS2D Acceptor-Lipophilic at lag 06	CATS 2D
3129 CATS2D 07 AL	CATS2D Acceptor-Lipophilic at lag 07	CATS 2D
3130 CATS2D 08 AL	CATS2D Acceptor-Lipophilic at lag 08	CATS 2D
3131 CATS2D_09_AL	CATS2D Acceptor-Lipophilic at lag 09	CATS 2D
3132 CATS2D_00_PP	CATS2D Positive-Positive at lag 00	CATS 2D
3133 CATS2D_01_PP	CATS2D Positive-Positive at lag 01	CATS 2D
3134 CATS2D_02_PP	CATS2D Positive-Positive at lag 02	CATS 2D
3135 CATS2D 03 PP	CATS2D Positive-Positive at lag 03	CATS 2D
3136 CATS2D_04_PP	CATS2D Positive-Positive at lag 04	CATS 2D
3137 CATS2D_05_PP	CATS2D Positive-Positive at lag 05	CATS 2D
3138 CATS2D_06_PP	CATS2D Positive-Positive at lag 06	CATS 2D
3139 CATS2D_07_PP	CATS2D Positive-Positive at lag 07	CATS 2D
3140 CATS2D_08_PP	CATS2D Positive-Positive at lag 08	CATS 2D
3141 CATS2D_09_PP	CATS2D Positive-Positive at lag 09	CATS 2D
3142 CATS2D_00_PN	CATS2D Positive-Negative at lag 00	CATS 2D
3143 CATS2D_01_PN	CATS2D Positive-Negative at lag 01	CATS 2D
3144 CATS2D_02_PN	CATS2D Positive-Negative at lag 02	CATS 2D
3145 CATS2D_03_PN	CATS2D Positive-Negative at lag 03	CATS 2D
3146 CATS2D_04_PN	CATS2D Positive-Negative at lag 04	CATS 2D
3147 CATS2D_05_PN	CATS2D Positive-Negative at lag 05	CATS 2D
3148 CATS2D_06_PN	CATS2D Positive-Negative at lag 06	CATS 2D
3149 CATS2D_07_PN	CATS2D Positive-Negative at lag 07	CATS 2D
3150 CATS2D_08_PN	CATS2D Positive-Negative at lag 08	CATS 2D
3151 CATS2D_09_PN	CATS2D Positive-Negative at lag 09	CATS 2D
3152 CATS2D_00_PL	CATS2D Positive Lipophilic at lag 00	CATS 2D
3153 CATS2D_01_PL	CATS2D Positive-Lipophilic at lag 01	CATS 2D
3154 CATS2D_02_PL	CATS2D Positive-Lipophilic at lag 02	CATS 2D
3155 CATS2D_03_PL	CATS2D Positive-Lipophilic at lag 03	CATS 2D
3156 CATS2D_04_PL	CATS2D Positive-Lipophilic at lag 04	CATS 2D
3157 CATS2D_05_PL	CATS2D Positive-Lipophilic at lag 05	CATS 2D
3158 CATS2D_06_PL	CATS2D Positive Lipophilic at lag 06	CATS 2D
3159 CATS2D_07_PL	CATS2D Positive-Lipophilic at lag 07	CATS 2D
3160 CATS2D_08_PL	CATS2D Positive-Lipophilic at lag 08	CATS 2D
3161 CATS2D_09_PL	CATS2D Positive-Lipophilic at lag 09	CATS 2D
3162 CATS2D_00_NN	CATS2D Negative Negative at lag 00	CATS 2D
3163 CATS2D_01_NN	CATS2D Negative-Negative at lag 01	CATS 2D
3164 CATS2D_02_NN	CATS2D Negative-Negative at lag 02	CATS 2D

3165 CATS2D_03_NN	CATS2D Negative-Negative at lag 03	CATS 2D
3166 CATS2D_04_NN	CATS2D Negative-Negative at lag 04	CATS 2D
3167 CATS2D_05_NN	CATS2D Negative-Negative at lag 05	CATS 2D
3168 CATS2D_06_NN	CATS2D Negative-Negative at lag 06	CATS 2D
3169 CATS2D 07 NN	CATS2D Negative-Negative at lag 07	CATS 2D
3170 CATS2D_08_NN	CATS2D Negative-Negative at lag 08	CATS 2D
3171 CATS2D 09 NN	CATS2D Negative-Negative at lag 09	CATS 2D
3172 CATS2D_00_NL	CATS2D Negative-Lipophilic at lag 00	CATS 2D
3173 CATS2D_01_NL	CATS2D Negative-Lipophilic at lag 01	CATS 2D
3174 CATS2D_02_NL	CATS2D Negative-Lipophilic at lag 02	CATS 2D
3175 CATS2D_03_NL	CATS2D Negative-Lipophilic at lag 03	CATS 2D
3176 CATS2D_04_NL	CATS2D Negative-Lipophilic at lag 04	CATS 2D
3177 CATS2D_05_NL	CATS2D Negative-Lipophilic at lag 05	CATS 2D
3178 CATS2D_06_NL	CATS2D Negative-Lipophilic at lag 06	CATS 2D
3179 CATS2D 07 NL	CATS2D Negative-Lipophilic at lag 07	CATS 2D
3180 CATS2D_08_NL	CATS2D Negative-Lipophilic at lag 08	CATS 2D
3181 CATS2D_09_NL	CATS2D Negative-Lipophilic at lag 09	CATS 2D
3182 CATS2D_00_LL	CATS2D Lipophilic-Lipophilic at lag 00	CATS 2D
3183 CATS2D_01_LL	CATS2D Lipophilic-Lipophilic at lag 01	CATS 2D
3184 CATS2D_02_LL	CATS2D Lipophilic-Lipophilic at lag 02	CATS 2D
3185 CATS2D_03_LL	CATS2D Lipophilic-Lipophilic at lag 03	CATS 2D
3186 CATS2D_04_LL	CATS2D Lipophilic-Lipophilic at lag 04	CATS 2D
3187 CATS2D_05_LL	CATS2D Lipophilic-Lipophilic at lag 05	CATS 2D
3188 CATS2D 06 LL	CATS2D Lipophilic-Lipophilic at lag 06	CATS 2D
3189 CATS2D_07_LL	CATS2D Lipophilic-Lipophilic at lag 07	CATS 2D
3190 CATS2D 08 LL	CATS2D Lipophilic-Lipophilic at lag 08	CATS 2D
3191 CATS2D 09 LL	CATS2D Lipophilic-Lipophilic at lag 09	CATS 2D
3192 T(NN)	sum of topological distances between NN	2D Atom Pairs
3193 T(NO)		2D Atom Pairs
	sum of topological distances between NO	
3194 T(NS)	sum of topological distances between NS	2D Atom Pairs
3195 T(NP)	sum of topological distances between NP	2D Atom Pairs
3196 T(NF)	sum of topological distances between NF	2D Atom Pairs
3197 T(NCI)	sum of topological distances between NCl	2D Atom Pairs
3198 T(NBr)	sum of topological distances between NBr	2D Atom Pairs
3199 T(NI)	sum of topological distances between NI	2D Atom Pairs
3200 T(OO)	sum of topological distances between OO	2D Atom Pairs
3201 T(OS)	sum of topological distances between OS	2D Atom Pairs
3202 T(OP)	sum of topological distances between OP	2D Atom Pairs
		2D Atom Pairs
3203 T(OF)	sum of topological distances between OF	
3204 T(OCl)	sum of topological distances between OCl	2D Atom Pairs
3205 T(OBr)	sum of topological distances between OBr	2D Atom Pairs
3206 T(OI)	sum of topological distances between OI	2D Atom Pairs
3207 T(SS)	sum of topological distances between SS	2D Atom Pairs
3208 T(SP)	sum of topological distances between SP	2D Atom Pairs
3209 T(SF)	sum of topological distances between SF	2D Atom Pairs
3210 T(SCI)	sum of topological distances between SCl	2D Atom Pairs
3211 T(SBr)	sum of topological distances between SBr	2D Atom Pairs
3212 T(SI)	sum of topological distances between SI	2D Atom Pairs
3213 T(PP)	sum of topological distances between PP	2D Atom Pairs
3214 T(PF)		
	sum of topological distances between PF	2D Atom Pairs
3215 T(PCI)	sum of topological distances between PCl	2D Atom Pairs
3216 T(PBr)	sum of topological distances between PBr	2D Atom Pairs
3217 T(PI)	sum of topological distances between PI	2D Atom Pairs
3218 T(FF)	sum of topological distances between FF	2D Atom Pairs
3219 T(FCI)	sum of topological distances between FCl	2D Atom Pairs
3220 T(FBr)	sum of topological distances between FBr	2D Atom Pairs
3221 T(FI)	sum of topological distances between FI	2D Atom Pairs
3222 T(CICI)	sum of topological distances between ClCl	2D Atom Pairs
3223 T(ClBr)	sum of topological distances between ClBr	2D Atom Pairs
3224 T(ClI)	sum of topological distances between ClI	2D Atom Pairs
	sum of topological distances between BrBr	2D Atom Pairs
3225 T(BrBr)	sum of topological distances between BrI	
3226 T(BrI)		2D Atom Pairs
3227 T(II)	sum of topological distances between II	2D Atom Pairs
3228 B01[C-C]	Presence/absence of C - C at topological distance 1	2D Atom Pairs
3229 B01[C-N]	Presence/absence of C - N at topological distance 1	2D Atom Pairs
3230 B01[C-O]	Presence/absence of C - O at topological distance 1	2D Atom Pairs
3231 B01[C-S]	Presence/absence of C - S at topological distance 1	2D Atom Pairs
3232 B01[C-P]	Presence/absence of C - P at topological distance 1	2D Atom Pairs
3233 B01[C-F]	Presence/absence of C - F at topological distance 1	2D Atom Pairs
3234 B01[C-CI]	Presence/absence of C - Cl at topological distance 1	2D Atom Pairs
3235 B01[C-Br]	Presence/absence of C - Br at topological distance 1	2D Atom Pairs
3236 B01[C-I]	Presence/absence of C - I at topological distance 1	2D Atom Pairs
3237 B01[C-B]	Presence/absence of C - B at topological distance 1	2D Atom Pairs
3238 B01[C-Si]	Presence/absence of C - Si at topological distance 1	2D Atom Pairs
3239 B01[C-X]	Presence/absence of C - X at topological distance 1	2D Atom Pairs
3240 B01[N-N]	Presence/absence of N - N at topological distance 1	2D Atom Pairs
		2D Atom Pairs
3241 B01[N-O]	Presence/absence of N - O at topological distance 1	2D Atom Pairs 2D Atom Pairs
3242 B01[N-S]	Presence/absence of N - S at topological distance 1	
3243 B01[N-P]	Presence/absence of N - P at topological distance 1	2D Atom Pairs
3244 B01[N-F]	Presence/absence of N - F at topological distance 1	2D Atom Pairs
3245 B01[N-CI]	Presence/absence of N - Cl at topological distance 1	2D Atom Pairs
3246 B01[N-Br]	Presence/absence of N - Br at topological distance 1	2D Atom Pairs
3247 B01[N-I]	Presence/absence of N - I at topological distance 1	2D Atom Pairs
3248 B01[N-B]	Presence/absence of N - B at topological distance 1	2D Atom Pairs
3249 B01[N-Si]	Presence/absence of N - Si at topological distance 1	2D Atom Pairs
3250 B01[N-X]	Presence/absence of N - X at topological distance 1	2D Atom Pairs
3251 B01[O-O]	Presence/absence of O - O at topological distance 1	2D Atom Pairs
3252 B01[O-S]	Presence/absence of O - S at topological distance 1	2D Atom Pairs
3253 B01[O-S]	Presence/absence of O - P at topological distance 1	2D Atom Pairs
3254 B01[O-F]	Presence/absence of O - F at topological distance 1	2D Atom Pairs
3255 B01[O-CI]	Presence/absence of 0 - Cl at topological distance 1	2D Atom Pairs
3256 B01[O-Br]	Presence/absence of O - Br at topological distance 1	2D Atom Pairs
3257 B01[O-I]	Presence/absence of O - I at topological distance 1	2D Atom Pairs
3258 B01[O-B]	Presence/absence of O - B at topological distance 1	2D Atom Pairs
3259 B01[O-Si]	Presence/absence of O - Si at topological distance 1	2D Atom Pairs
3260 B01[O-X]	Presence/absence of O - X at topological distance 1	2D Atom Pairs



3261	B01[S-S]	Presence/absence of S - S at topological distance 1	2D Atom Pairs
	B01[S-P]		2D Atom Pairs
	B01[S-F]		2D Atom Pairs
	B01[S-CI]	· ·	2D Atom Pairs
	B01[S-Br]		2D Atom Pairs
	B01[S-I]		2D Atom Pairs
	B01[S-B]		2D Atom Pairs
3268	B01[S-Si]		2D Atom Pairs
3269	B01[S-X]	Presence/absence of S - X at topological distance 1	2D Atom Pairs
3270	B01[P-P]	Presence/absence of P - P at topological distance 1	2D Atom Pairs
	B01[P-F]		2D Atom Pairs
	B01[P-CI]	· ·	2D Atom Pairs
			2D Atom Pairs
	B01[P-Br]		
	B01[P-I]	. •	2D Atom Pairs
	B01[P-B]		2D Atom Pairs
3276	B01[P-Si]	Presence/absence of P - Si at topological distance 1	2D Atom Pairs
3277	B01[P-X]	Presence/absence of P - X at topological distance 1	2D Atom Pairs
3278	B01[F-F]	Presence/absence of F - F at topological distance 1	2D Atom Pairs
	B01[F-CI]	Presence/absence of F - Cl at topological distance 1	2D Atom Pairs
	B01[F-Br]		2D Atom Pairs
	B01[F-I]		2D Atom Pairs
	B01[F-B]	, ,	2D Atom Pairs
3283	B01[F-Si]	Presence/absence of F - Si at topological distance 1	2D Atom Pairs
3284	B01[F-X]	Presence/absence of F - X at topological distance 1	2D Atom Pairs
3285	B01[CI-CI]	Presence/absence of CI - CI at topological distance 1	2D Atom Pairs
3286	B01[CI-Br]	Presence/absence of CI - Br at topological distance 1	2D Atom Pairs
	B01[CI-I]		2D Atom Pairs
	B01[CI-B]		2D Atom Pairs
			2D Atom Pairs
	B01[CI-Si]	, ,	
	B01[CI-X]	. *	2D Atom Pairs
	B01[Br-Br]		2D Atom Pairs
3292	B01[Br-I]	Presence/absence of Br - I at topological distance 1	2D Atom Pairs
3293	B01[Br-B]	Presence/absence of Br - B at topological distance 1	2D Atom Pairs
	B01[Br-Si]		2D Atom Pairs
	B01[Br-X]		2D Atom Pairs
	B01[I-I]	, ,	2D Atom Pairs
			2D Atom Pairs
	B01[I-B]		
	B01[I-Si]		2D Atom Pairs
3299	B01[I-X]	Presence/absence of I - X at topological distance 1	2D Atom Pairs
3300	B01[B-B]	Presence/absence of B - B at topological distance 1	2D Atom Pairs
3301	B01[B-Si]	Presence/absence of B - Si at topological distance 1	2D Atom Pairs
	B01[B-X]		2D Atom Pairs
	B01[Si-Si]		2D Atom Pairs
	B01[Si-X]		2D Atom Pairs
	B01[X-X]		2D Atom Pairs
	B02[C-C]	. •	2D Atom Pairs
3307	B02[C-N]	Presence/absence of C - N at topological distance 2	2D Atom Pairs
3308	B02[C-O]	Presence/absence of C - O at topological distance 2	2D Atom Pairs
3309	B02[C-S]	Presence/absence of C - S at topological distance 2	2D Atom Pairs
3310	B02[C-P]		2D Atom Pairs
	B02[C-F]	, ,	2D Atom Pairs
	B02[C-CI]		2D Atom Pairs
	B02[C-Br]		2D Atom Pairs
	B02[C-I]	, ,	2D Atom Pairs
3315	B02[C-B]	Presence/absence of C - B at topological distance 2	2D Atom Pairs
	B02[C-Si]	Presence/absence of C - Si at topological distance 2	2D Atom Pairs
3317	B02[C-X]	Presence/absence of C - X at topological distance 2	2D Atom Pairs
	B02[N-N]		2D Atom Pairs
	B02[N-O]		2D Atom Pairs
	B02[N-S]		2D Atom Pairs
	B02[N-P]		2D Atom Pairs
	B02[N-F]		2D Atom Pairs
	B02[N-CI]		2D Atom Pairs
	B02[N-Br]		2D Atom Pairs
3325	B02[N-I]	Presence/absence of N - I at topological distance 2	2D Atom Pairs
	B02[N-B]		2D Atom Pairs
	B02[N-Si]		2D Atom Pairs
	B02[N-X]		2D Atom Pairs
	B02[O-O]		2D Atom Pairs
	B02[O-S]	·	2D Atom Pairs
			2D Atom Pairs
	B02[O-P]		
	B02[O-F]		2D Atom Pairs
	B02[O-CI]		2D Atom Pairs
	B02[O-Br]		2D Atom Pairs
3335	B02[O-I]	Presence/absence of O - I at topological distance 2	2D Atom Pairs
	B02[O-B]		2D Atom Pairs
	B02[O-Si]		2D Atom Pairs
	B02[O-X]		2D Atom Pairs
	B02[S-S]		2D Atom Pairs
		· · · · · · · · · · · · · · · · · · ·	
	B02[S-P]		2D Atom Pairs
	B02[S-F]		2D Atom Pairs
	B02[S-CI]		2D Atom Pairs
3343	B02[S-Br]	Presence/absence of S - Br at topological distance 2	2D Atom Pairs
	B02[S-I]		2D Atom Pairs
	B02[S-B]		2D Atom Pairs
	B02[S-Si]		2D Atom Pairs
	B02[S-X]		2D Atom Pairs
	B02[P-P]	. •	2D Atom Pairs
	B02[P-F]		2D Atom Pairs
	B02[P-CI]		2D Atom Pairs
3351	B02[P-Br]	Presence/absence of P - Br at topological distance 2	2D Atom Pairs
	B02[P-I]		2D Atom Pairs
	B02[P-B]		2D Atom Pairs
	B02[P-Si]		2D Atom Pairs
	B02[P-X]		2D Atom Pairs
	B02[F-K]		2D Atom Pairs
2300			ans



	B02[F-CI]	Presence/absence of F - CI at topological distance 2	2D Atom Pairs
	B02[F-Br]	Presence/absence of F - Br at topological distance 2	2D Atom Pairs
	B02[F-I]	Presence/absence of F - I at topological distance 2	2D Atom Pairs
	B02[F-B]	Presence/absence of F - B at topological distance 2	2D Atom Pairs
	B02[F-Si]	Presence/absence of F - Si at topological distance 2	2D Atom Pairs
	B02[F-X]	Presence/absence of F - X at topological distance 2	2D Atom Pairs
	B02[CI-CI]	Presence/absence of CI - CI at topological distance 2	2D Atom Pairs
	B02[CI-Br]	Presence/absence of CI - Br at topological distance 2	2D Atom Pairs 2D Atom Pairs
	B02[CI-I]	Presence/absence of CL - Lat topological distance 2	
	B02[CI-B]	Presence/absence of CI - B at topological distance 2 Presence/absence of CI - Si at topological distance 2	2D Atom Pairs 2D Atom Pairs
	B02[CI-Si] B02[CI-X]	Presence/absence of CI - X at topological distance 2	2D Atom Pairs
	B02[Br-Br]	Presence/absence of Br - Br at topological distance 2	2D Atom Pairs
	B02[Br-I]	Presence/absence of Br - I at topological distance 2	2D Atom Pairs
	B02[Br-B]	Presence/absence of Br - B at topological distance 2	2D Atom Pairs
	B02[Br-Si]	Presence/absence of Br - Si at topological distance 2	2D Atom Pairs
	B02[Br-X]	Presence/absence of Br - X at topological distance 2	2D Atom Pairs
	B02[I-I]	Presence/absence of I - I at topological distance 2	2D Atom Pairs
	B02[I-B]	Presence/absence of I - B at topological distance 2	2D Atom Pairs
	B02[I-Si]	Presence/absence of I - Si at topological distance 2	2D Atom Pairs
	B02[I-X]	Presence/absence of I - X at topological distance 2	2D Atom Pairs
	B02[B-B]	Presence/absence of B - B at topological distance 2	2D Atom Pairs
3379	B02[B-Si]	Presence/absence of B - Si at topological distance 2	2D Atom Pairs
3380	B02[B-X]	Presence/absence of B - X at topological distance 2	2D Atom Pairs
3381	B02[Si-Si]	Presence/absence of Si - Si at topological distance 2	2D Atom Pairs
	B02[Si-X]	Presence/absence of Si - X at topological distance 2	2D Atom Pairs
	B02[X-X]	Presence/absence of X - X at topological distance 2	2D Atom Pairs
	B03[C-C]	Presence/absence of C - C at topological distance 3	2D Atom Pairs
	B03[C-N]	Presence/absence of C - N at topological distance 3	2D Atom Pairs
	B03[C-O]	Presence/absence of C - O at topological distance 3	2D Atom Pairs
	B03[C-S]	Presence/absence of C - S at topological distance 3	2D Atom Pairs
	B03[C-P]	Presence/absence of C - P at topological distance 3	2D Atom Pairs
	B03[C-F]	Presence/absence of C - F at topological distance 3	2D Atom Pairs 2D Atom Pairs
	B03[C-CI]	Presence/absence of C - Cl at topological distance 3	
	B03[C-Br] B03[C-I]	Presence/absence of C - Br at topological distance 3	2D Atom Pairs 2D Atom Pairs
	B03[C-I]	Presence/absence of C - I at topological distance 3 Presence/absence of C - B at topological distance 3	2D Atom Pairs
	B03[C-Si]	Presence/absence of C - Si at topological distance 3	2D Atom Pairs
	B03[C-X]	Presence/absence of C - X at topological distance 3	2D Atom Pairs
	B03[N-N]	Presence/absence of N - N at topological distance 3	2D Atom Pairs
	B03[N-O]	Presence/absence of N - O at topological distance 3	2D Atom Pairs
	B03[N-S]	Presence/absence of N - S at topological distance 3	2D Atom Pairs
	B03[N-P]	Presence/absence of N - P at topological distance 3	2D Atom Pairs
	B03[N-F]	Presence/absence of N - F at topological distance 3	2D Atom Pairs
	B03[N-CI]	Presence/absence of N - Cl at topological distance 3	2D Atom Pairs
	B03[N-Br]	Presence/absence of N - Br at topological distance 3	2D Atom Pairs
	B03[N-I]	Presence/absence of N - I at topological distance 3	2D Atom Pairs
3404	B03[N-B]	Presence/absence of N - B at topological distance 3	2D Atom Pairs
3405	B03[N-Si]	Presence/absence of N - Si at topological distance 3	2D Atom Pairs
	B03[N-X]	Presence/absence of N - X at topological distance 3	2D Atom Pairs
	B03[O-O]	Presence/absence of O - O at topological distance 3	2D Atom Pairs
	B03[O-S]	Presence/absence of O - S at topological distance 3	2D Atom Pairs
	B03[O-P]	Presence/absence of O - P at topological distance 3	2D Atom Pairs
	B03[O-F]	Presence/absence of O - F at topological distance 3	2D Atom Pairs
	B03[O-CI] B03[O-Br]	Presence/absence of O - Cl at topological distance 3 Presence/absence of O - Br at topological distance 3	2D Atom Pairs 2D Atom Pairs
	B03[O-I]	Presence/absence of O - I at topological distance 3	2D Atom Pairs
	B03[O-B]	Presence/absence of O - B at topological distance 3	2D Atom Pairs
	B03[O-Si]	Presence/absence of O - Si at topological distance 3	2D Atom Pairs
	B03[O-X]	Presence/absence of O - X at topological distance 3	2D Atom Pairs
	B03[S-S]	Presence/absence of S - S at topological distance 3	2D Atom Pairs
	B03[S-P]	Presence/absence of S - P at topological distance 3	2D Atom Pairs
	B03[S-F]	Presence/absence of S - F at topological distance 3	2D Atom Pairs
	B03[S-CI]	Presence/absence of S - Cl at topological distance 3	2D Atom Pairs
3421	B03[S-Br]	Presence/absence of S - Br at topological distance 3	2D Atom Pairs
3422	B03[S-I]	Presence/absence of S - I at topological distance 3	2D Atom Pairs
	B03[S-B]	Presence/absence of S - B at topological distance 3	2D Atom Pairs
	B03[S-Si]	Presence/absence of S - Si at topological distance 3	2D Atom Pairs
	B03[S-X]	Presence/absence of S - X at topological distance 3	2D Atom Pairs
	B03[P-P]	Presence/absence of P - P at topological distance 3	2D Atom Pairs
	B03[P-F]	Presence/absence of P - F at topological distance 3	2D Atom Pairs
	B03[P-CI]	Presence/absence of P - Cl at topological distance 3	2D Atom Pairs
	B03[P-Br]	Presence/absence of P - Br at topological distance 3	2D Atom Pairs
	B03[P-I]	Presence/absence of P - I at topological distance 3 Presence/absence of P - B at topological distance 3	2D Atom Pairs 2D Atom Pairs
	B03[P-B] B03[P-Si]		2D Atom Pairs
	B03[P-X]	Presence/absence of P - Si at topological distance 3 Presence/absence of P - X at topological distance 3	2D Atom Pairs
	B03[F-F]	Presence/absence of F - F at topological distance 3	2D Atom Pairs
	B03[F-CI]	Presence/absence of F - Cl at topological distance 3	2D Atom Pairs
	B03[F-Br]	Presence/absence of F - Br at topological distance 3	2D Atom Pairs
	B03[F-I]	Presence/absence of F - I at topological distance 3	2D Atom Pairs
	B03[F-B]	Presence/absence of F - B at topological distance 3	2D Atom Pairs
	B03[F-Si]	Presence/absence of F - Si at topological distance 3	2D Atom Pairs
3440	B03[F-X]	Presence/absence of F - X at topological distance 3	2D Atom Pairs
3441	B03[CI-CI]	Presence/absence of CI - CI at topological distance 3	2D Atom Pairs
	B03[Cl-Br]	Presence/absence of CI - Br at topological distance 3	2D Atom Pairs
	B03[CI-I]	Presence/absence of CI - I at topological distance 3	2D Atom Pairs
	B03[CI-B]	Presence/absence of CI - B at topological distance 3	2D Atom Pairs
	B03[CI-Si]	Presence/absence of CI - Si at topological distance 3	2D Atom Pairs
	B03[CI-X]	Presence/absence of CI - X at topological distance 3	2D Atom Pairs
	B03[Br-Br]	Presence/absence of Br - Br at topological distance 3	2D Atom Pairs
	B03[Br-I]	Presence/absence of Br - I at topological distance 3	2D Atom Pairs
	B03[Br-B] B03[Br-Si]	Presence/absence of Br - B at topological distance 3 Presence/absence of Br - Si at topological distance 3	2D Atom Pairs 2D Atom Pairs
	B03[Br-X]	Presence/absence of Br - X at topological distance 3	2D Atom Pairs
	B03[I-I]	Presence/absence of I - I at topological distance 3	2D Atom Pairs
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3453	B03[I-B]	Presence/absence of I - B at topological distance 3	2D Atom Pairs
3454	B03[I-Si]	Presence/absence of I - Si at topological distance 3	2D Atom Pairs
	B03[I-X]		2D Atom Pairs
	B03[B-B]	Presence/absence of B - B at topological distance 3	2D Atom Pairs
		. •	
	B03[B-Si]	Presence/absence of B - Si at topological distance 3	2D Atom Pairs
	B03[B-X]	Presence/absence of B - X at topological distance 3	2D Atom Pairs
	B03[Si-Si]	Presence/absence of Si - Si at topological distance 3	2D Atom Pairs
3460	B03[Si-X]	Presence/absence of Si - X at topological distance 3	2D Atom Pairs
	B03[X-X]	Presence/absence of X - X at topological distance 3	2D Atom Pairs
	B04[C-C]	Presence/absence of C - C at topological distance 4	2D Atom Pairs
3463	B04[C-N]		2D Atom Pairs
3464	B04[C-O]	Presence/absence of C - O at topological distance 4	2D Atom Pairs
3465	B04[C-S]	Presence/absence of C - S at topological distance 4	2D Atom Pairs
	B04[C-P]		2D Atom Pairs
	B04[C-F]	Presence/absence of C - F at topological distance 4	2D Atom Pairs
3468	B04[C-CI]	Presence/absence of C - Cl at topological distance 4	2D Atom Pairs
3469	B04[C-Br]	Presence/absence of C - Br at topological distance 4	2D Atom Pairs
3470	B04[C-I]	Presence/absence of C - I at topological distance 4	2D Atom Pairs
	B04[C-B]	Presence/absence of C - B at topological distance 4	2D Atom Pairs
	B04[C-Si]	, ,	2D Atom Pairs
3473	B04[C-X]	Presence/absence of C - X at topological distance 4	2D Atom Pairs
3474	B04[N-N]	Presence/absence of N - N at topological distance 4	2D Atom Pairs
	B04[N-O]		2D Atom Pairs
	B04[N-S]		2D Atom Pairs
	B04[N-P]	Presence/absence of N - P at topological distance 4	2D Atom Pairs
3478	B04[N-F]		2D Atom Pairs
3479	B04[N-CI]	Presence/absence of N - Cl at topological distance 4	2D Atom Pairs
	B04[N-Br]	Presence/absence of N - Br at topological distance 4	2D Atom Pairs
	B04[N-I]	Presence/absence of N - I at topological distance 4	2D Atom Pairs
	B04[N-B]		2D Atom Pairs
		. •	
	B04[N-Si]		2D Atom Pairs
	B04[N-X]	Presence/absence of N - X at topological distance 4	2D Atom Pairs
3485	B04[O-O]	Presence/absence of O - O at topological distance 4	2D Atom Pairs
	B04[O-S]	Presence/absence of O - S at topological distance 4	2D Atom Pairs
	B04[O-P]		2D Atom Pairs
	B04[O-F]		2D Atom Pairs
3489	B04[O-CI]		2D Atom Pairs
3490	B04[O-Br]	Presence/absence of O - Br at topological distance 4	2D Atom Pairs
3491	B04[O-I]	Presence/absence of O - I at topological distance 4	2D Atom Pairs
	B04[O-B]		2D Atom Pairs
	B04[O-Si]	Presence/absence of O - Si at topological distance 4	2D Atom Pairs
3494	B04[O-X]		2D Atom Pairs
3495	B04[S-S]	Presence/absence of S - S at topological distance 4	2D Atom Pairs
3496	B04[S-P]	Presence/absence of S - P at topological distance 4	2D Atom Pairs
	B04[S-F]	Presence/absence of S - F at topological distance 4	2D Atom Pairs
	B04[S-CI]	, ,	2D Atom Pairs
	B04[S-Br]	Presence/absence of S - Br at topological distance 4	2D Atom Pairs
3500	B04[S-I]	Presence/absence of S - I at topological distance 4	2D Atom Pairs
3501	B04[S-B]	Presence/absence of S - B at topological distance 4	2D Atom Pairs
	B04[S-Si]	Presence/absence of S - Si at topological distance 4	2D Atom Pairs
	B04[S-X]	Presence/absence of S - X at topological distance 4	2D Atom Pairs
	B04[P-P]		2D Atom Pairs
3505	B04[P-F]	Presence/absence of P - F at topological distance 4	2D Atom Pairs
3506	B04[P-CI]	Presence/absence of P - Cl at topological distance 4	2D Atom Pairs
3507	B04[P-Br]	Presence/absence of P - Br at topological distance 4	2D Atom Pairs
	B04[P-I]		2D Atom Pairs
	B04[P-B]		2D Atom Pairs
		Presence/absence of P - B at topological distance 4	
	B04[P-Si]		2D Atom Pairs
3511	B04[P-X]	Presence/absence of P - X at topological distance 4	2D Atom Pairs
3512	B04[F-F]	Presence/absence of F - F at topological distance 4	2D Atom Pairs
	B04[F-CI]		2D Atom Pairs
	B04[F-Br]	Presence/absence of F - Br at topological distance 4	2D Atom Pairs
	B04[F-B]	Presence/absence of F - I at topological distance 4	2D Atom Pairs
	B04[F-B]	Presence/absence of F - B at topological distance 4	2D Atom Pairs
3517	B04[F-Si]	Presence/absence of F - Si at topological distance 4	2D Atom Pairs
3518	B04[F-X]	Presence/absence of F - X at topological distance 4	2D Atom Pairs
	B04[CI-CI]		2D Atom Pairs
	B04[CI-Br]		2D Atom Pairs
			2D Atom Pairs
	B04[CI-I]	Presence/absence of CI - I at topological distance 4	
	B04[CI-B]	Presence/absence of CI - B at topological distance 4	2D Atom Pairs
3523	B04[CI-Si]		2D Atom Pairs
3524	B04[CI-X]	Presence/absence of CI - X at topological distance 4	2D Atom Pairs
	B04[Br-Br]	Presence/absence of Br - Br at topological distance 4	2D Atom Pairs
	B04[Br-I]		2D Atom Pairs
	B04[Br-B]		2D Atom Pairs
	B04[Br-Si]	Presence/absence of Br - Si at topological distance 4	2D Atom Pairs
3529	B04[Br-X]	Presence/absence of Br - X at topological distance 4	2D Atom Pairs
3530	B04[I-I]	Presence/absence of I - I at topological distance 4	2D Atom Pairs
	B04[I-B]		2D Atom Pairs
	B04[I-Si]		2D Atom Pairs
	B04[I-X]	Presence/absence of I - X at topological distance 4	2D Atom Pairs
	B04[B-B]	Presence/absence of B - B at topological distance 4	2D Atom Pairs
3535	B04[B-Si]	Presence/absence of B - Si at topological distance 4	2D Atom Pairs
	B04[B-X]	Presence/absence of B - X at topological distance 4	2D Atom Pairs
	B04[Si-Si]	Presence/absence of Si - Si at topological distance 4	2D Atom Pairs
		Presence/absence of Si - X at topological distance 4	
	B04[Si-X]		2D Atom Pairs
	B04[X-X]		2D Atom Pairs
3540	B05[C-C]	Presence/absence of C - C at topological distance 5	2D Atom Pairs
	B05[C-N]	Presence/absence of C - N at topological distance 5	2D Atom Pairs
	B05[C-O]	Presence/absence of C - O at topological distance 5	2D Atom Pairs
	B05[C-S]	Presence/absence of C - S at topological distance 5	2D Atom Pairs
	B05[C-P]	Presence/absence of C - P at topological distance 5	2D Atom Pairs
	B05[C-F]		2D Atom Pairs
3546	B05[C-CI]		2D Atom Pairs
	B05[C-Br]	Presence/absence of C - Br at topological distance 5	2D Atom Pairs
	B05[C-I]	Presence/absence of C - I at topological distance 5	2D Atom Pairs
20-10	[- 1]		



3549	B05[C-B]	Presence/absence of C - B at topological distance 5	2D Atom Pairs
	B05[C-Si]	Presence/absence of C - Si at topological distance 5	2D Atom Pairs
	B05[C-X]		2D Atom Pairs
	B05[N-N]		2D Atom Pairs
	B05[N-O]	. •	2D Atom Pairs
	B05[N-S]		2D Atom Pairs
3555	B05[N-P]		2D Atom Pairs
3556	B05[N-F]	Presence/absence of N - F at topological distance 5	2D Atom Pairs
	B05[N-CI]	Presence/absence of N - Cl at topological distance 5	2D Atom Pairs
	B05[N-Br]		2D Atom Pairs
	B05[N-I]		2D Atom Pairs
	B05[N-B]		2D Atom Pairs
	B05[N-Si]		2D Atom Pairs
3562	B05[N-X]	Presence/absence of N - X at topological distance 5	2D Atom Pairs
3563	B05[O-O]	Presence/absence of O - O at topological distance 5	2D Atom Pairs
	B05[O-S]	Presence/absence of O - S at topological distance 5	2D Atom Pairs
	B05[O-P]		2D Atom Pairs
			2D Atom Pairs
	B05[O-F]		
	B05[O-CI]	. •	2D Atom Pairs
3568	B05[O-Br]	Presence/absence of O - Br at topological distance 5	2D Atom Pairs
3569	B05[O-I]	Presence/absence of O - I at topological distance 5	2D Atom Pairs
3570	B05[O-B]	Presence/absence of O - B at topological distance 5	2D Atom Pairs
	B05[O-Si]		2D Atom Pairs
			2D Atom Pairs
	B05[O-X]	, ,	
	B05[S-S]		2D Atom Pairs
	B05[S-P]		2D Atom Pairs
3575	B05[S-F]	Presence/absence of S - F at topological distance 5	2D Atom Pairs
3576	B05[S-CI]	Presence/absence of S - Cl at topological distance 5	2D Atom Pairs
3577	B05[S-Br]		2D Atom Pairs
	B05[S-I]		2D Atom Pairs
	B05[S-B]		2D Atom Pairs
3580	B05[S-Si]		2D Atom Pairs
3581	B05[S-X]	Presence/absence of S - X at topological distance 5	2D Atom Pairs
3582	B05[P-P]	Presence/absence of P - P at topological distance 5	2D Atom Pairs
	B05[P-F]		2D Atom Pairs
	B05[P-CI]		2D Atom Pairs
	B05[P-Br]		2D Atom Pairs
3586	B05[P-I]		2D Atom Pairs
3587	B05[P-B]	Presence/absence of P - B at topological distance 5	2D Atom Pairs
3588	B05[P-Si]	Presence/absence of P - Si at topological distance 5	2D Atom Pairs
	B05[P-X]		2D Atom Pairs
	B05[F-F]	· ·	2D Atom Pairs
	B05[F-CI]		2D Atom Pairs
	B05[F-Br]		2D Atom Pairs
3593	B05[F-I]	Presence/absence of F - I at topological distance 5	2D Atom Pairs
3594	B05[F-B]	Presence/absence of F - B at topological distance 5	2D Atom Pairs
	B05[F-Si]		2D Atom Pairs
	B05[F-X]		2D Atom Pairs
	B05[CI-CI]	·	2D Atom Pairs
	B05[CI-Br]	· ·	2D Atom Pairs
3599	B05[CI-I]	Presence/absence of CI - I at topological distance 5	2D Atom Pairs
3600	B05[CI-B]	Presence/absence of Cl - B at topological distance 5	2D Atom Pairs
	B05[CI-Si]		2D Atom Pairs
	B05[CI-X]		2D Atom Pairs
		, ,	2D Atom Pairs
	B05[Br-Br]	· · · · · · · · · · · · · · · · · · ·	
	B05[Br-I]		2D Atom Pairs
3605	B05[Br-B]	Presence/absence of Br - B at topological distance 5	2D Atom Pairs
3606	B05[Br-Si]	Presence/absence of Br - Si at topological distance 5	2D Atom Pairs
3607	B05[Br-X]	Presence/absence of Br - X at topological distance 5	2D Atom Pairs
	B05[I-I]		2D Atom Pairs
			2D Atom Pairs
	B05[I-B]		
	B05[I-Si]		2D Atom Pairs
	B05[I-X]		2D Atom Pairs
	B05[B-B]		2D Atom Pairs
3613	B05[B-Si]	Presence/absence of B - Si at topological distance 5	2D Atom Pairs
	B05[B-X]		2D Atom Pairs
	B05[Si-Si]		2D Atom Pairs
	B05[Si-X]		2D Atom Pairs
	B05[X-X]		2D Atom Pairs
	B06[C-C]		2D Atom Pairs
3619	B06[C-N]	Presence/absence of C - N at topological distance 6	2D Atom Pairs
3620	B06[C-O]	Presence/absence of C - O at topological distance 6	2D Atom Pairs
	B06[C-S]		2D Atom Pairs
	B06[C-P]		2D Atom Pairs
			2D Atom Pairs
	B06[C-F]		
	B06[C-CI]		2D Atom Pairs
	B06[C-Br]		2D Atom Pairs
	B06[C-I]		2D Atom Pairs
3627	B06[C-B]	Presence/absence of C - B at topological distance 6	2D Atom Pairs
	B06[C-Si]		2D Atom Pairs
	B06[C-X]		2D Atom Pairs
	B06[N-N]	. •	2D Atom Pairs
	B06[N-O]		2D Atom Pairs
	B06[N-S]		2D Atom Pairs
	B06[N-P]	Presence/absence of N - P at topological distance 6	2D Atom Pairs
	B06[N-F]		2D Atom Pairs
	B06[N-CI]		2D Atom Pairs
			2D Atom Pairs
	B06[N-Br]	. •	
	B06[N-I]		2D Atom Pairs
3638	B06[N-B]		2D Atom Pairs
3639	B06[N-Si]		2D Atom Pairs
	B06[N-X]		2D Atom Pairs
	B06[O-O]		2D Atom Pairs
	B06[O-S]		2D Atom Pairs
	B06[O-P]		2D Atom Pairs
3644	B06[O-F]	Presence/absence of O - F at topological distance 6	2D Atom Pairs



3645	B06[O-CI]	Presence/absence of O - Cl at topological distance 6	2D Atom Pairs
3646	B06[O-Br]	Presence/absence of O - Br at topological distance 6	2D Atom Pairs
	B06[O-I]		2D Atom Pairs
	B06[O-B]		2D Atom Pairs
	B06[O-Si]	, ,	2D Atom Pairs
	B06[O-X]		2D Atom Pairs
	B06[S-S]	Presence/absence of S - S at topological distance 6	2D Atom Pairs
3652	B06[S-P]	Presence/absence of S - P at topological distance 6	2D Atom Pairs
	B06[S-F]		2D Atom Pairs
	B06[S-CI]		2D Atom Pairs
	B06[S-Br]		
			2D Atom Pairs
	B06[S-I]		2D Atom Pairs
3657	B06[S-B]	Presence/absence of S - B at topological distance 6	2D Atom Pairs
3658	B06[S-Si]	Presence/absence of S - Si at topological distance 6	2D Atom Pairs
	B06[S-X]		2D Atom Pairs
			2D Atom Pairs
	B06[P-P]	. •	
	B06[P-F]		2D Atom Pairs
3662	B06[P-CI]	Presence/absence of P - Cl at topological distance 6	2D Atom Pairs
3663	B06[P-Br]	Presence/absence of P - Br at topological distance 6	2D Atom Pairs
	B06[P-I]	Presence/absence of P - I at topological distance 6	2D Atom Pairs
	B06[P-B]		2D Atom Pairs
	B06[P-Si]		2D Atom Pairs
3667	B06[P-X]		2D Atom Pairs
3668	B06[F-F]	Presence/absence of F - F at topological distance 6	2D Atom Pairs
3669	B06[F-CI]	Presence/absence of F - Cl at topological distance 6	2D Atom Pairs
	B06[F-Br]		2D Atom Pairs
	B06[F-I]		2D Atom Pairs
	B06[F-B]	, ,	2D Atom Pairs
	B06[F-Si]	. •	2D Atom Pairs
3674	B06[F-X]	Presence/absence of F - X at topological distance 6	2D Atom Pairs
	B06[CI-CI]	Presence/absence of CI - CI at topological distance 6	2D Atom Pairs
	B06[CI-Br]		2D Atom Pairs
	B06[CI-I]	· · · · · · · · · · · · · · · · · · ·	2D Atom Pairs
	B06[CI-B]	, ,	2D Atom Pairs
	B06[CI-Si]	, ,	2D Atom Pairs
3680	B06[CI-X]	Presence/absence of Cl - X at topological distance 6	2D Atom Pairs
	B06[Br-Br]		2D Atom Pairs
	B06[Br-I]		2D Atom Pairs
			2D Atom Pairs
	B06[Br-B]	, ,	
	B06[Br-Si]	·	2D Atom Pairs
3685	B06[Br-X]	Presence/absence of Br - X at topological distance 6	2D Atom Pairs
3686	B06[I-I]	Presence/absence of I - I at topological distance 6	2D Atom Pairs
3687	B06[I-B]	Presence/absence of I - B at topological distance 6	2D Atom Pairs
	B06[I-Si]		2D Atom Pairs
	B06[I-X]		2D Atom Pairs
	B06[B-B]		2D Atom Pairs
		. •	
	B06[B-Si]	·	2D Atom Pairs
	B06[B-X]	Presence/absence of B - X at topological distance 6	2D Atom Pairs
3693	B06[Si-Si]	Presence/absence of Si - Si at topological distance 6	2D Atom Pairs
3694	B06[Si-X]	Presence/absence of Si - X at topological distance 6	2D Atom Pairs
3695	B06[X-X]	Presence/absence of X - X at topological distance 6	2D Atom Pairs
	B07[C-C]		2D Atom Pairs
	B07[C-N]		2D Atom Pairs
			2D Atom Pairs
	B07[C-O]		
	B07[C-S]	· ·	2D Atom Pairs
	B07[C-P]	Presence/absence of C - P at topological distance 7	2D Atom Pairs
3701	B07[C-F]	Presence/absence of C - F at topological distance 7	2D Atom Pairs
	B07[C-CI]	Presence/absence of C - Cl at topological distance 7	2D Atom Pairs
	B07[C-Br]		2D Atom Pairs
	B07[C-I]	,	2D Atom Pairs
	B07[C-B]		2D Atom Pairs
	B07[C-Si]		2D Atom Pairs
3707	B07[C-X]	Presence/absence of C - X at topological distance 7	2D Atom Pairs
	B07[N-N]		2D Atom Pairs
	B07[N-O]		2D Atom Pairs
		. •	2D Atom Pairs
	B07[N-S]		
	B07[N-P]		2D Atom Pairs
	B07[N-F]		2D Atom Pairs
3713	B07[N-CI]		2D Atom Pairs
	B07[N-Br]	Presence/absence of N - Br at topological distance 7	2D Atom Pairs
	B07[N-I]		2D Atom Pairs
	B07[N-B]		2D Atom Pairs
	B07[N-Si]		2D Atom Pairs
	B07[N-X]		2D Atom Pairs
3719	B07[O-O]	Presence/absence of O - O at topological distance 7	2D Atom Pairs
3720	B07[O-S]	Presence/absence of O - S at topological distance 7	2D Atom Pairs
	B07[O-P]		2D Atom Pairs
	B07[O-F]		2D Atom Pairs
	B07[O-CI]		2D Atom Pairs
	B07[O-Br]		2D Atom Pairs
	B07[O-I]		2D Atom Pairs
	B07[O-B]		2D Atom Pairs
3727	B07[O-Si]	Presence/absence of O - Si at topological distance 7	2D Atom Pairs
	B07[O-X]		2D Atom Pairs
	B07[S-S]		2D Atom Pairs
	B07[S-P]		2D Atom Pairs
			2D Atom Pairs
	B07[S-F]		
	B07[S-CI]		2D Atom Pairs
	B07[S-Br]		2D Atom Pairs
	B07[S-I]		2D Atom Pairs
	B07[S-B]	Presence/absence of S - B at topological distance 7	2D Atom Pairs
	B07[S-Si]		2D Atom Pairs
	B07[S-X]		2D Atom Pairs
			2D Atom Pairs
	B07[P-P]		
	B07[P-F]		2D Atom Pairs
3740	B07[P-CI]	Presence/absence of P - Cl at topological distance 7	2D Atom Pairs



3741	B07[P-Br]	Presence/absence of P - Br at topological distance 7	2D Atom Pairs
3742	B07[P-I]		2D Atom Pairs
	B07[P-B]		2D Atom Pairs
	B07[P-Si]	· ·	2D Atom Pairs
	B07[P-X]		2D Atom Pairs
	B07[F-F]		2D Atom Pairs
3747	B07[F-CI]	Presence/absence of F - Cl at topological distance 7	2D Atom Pairs
3748	B07[F-Br]	Presence/absence of F - Br at topological distance 7	2D Atom Pairs
	B07[F-I]		2D Atom Pairs
	B07[F-B]		2D Atom Pairs
			2D Atom Pairs
	B07[F-Si]		
	B07[F-X]		2D Atom Pairs
3753	B07[CI-CI]	Presence/absence of CI - CI at topological distance 7	2D Atom Pairs
3754	B07[CI-Br]	Presence/absence of CI - Br at topological distance 7	2D Atom Pairs
3755	B07[CI-I]	Presence/absence of CI - I at topological distance 7	2D Atom Pairs
	B07[CI-B]		2D Atom Pairs
	B07[CI-Si]		2D Atom Pairs
	B07[CI-X]		2D Atom Pairs
3759	B07[Br-Br]		2D Atom Pairs
3760	B07[Br-I]	Presence/absence of Br - I at topological distance 7	2D Atom Pairs
3761	B07[Br-B]	Presence/absence of Br - B at topological distance 7	2D Atom Pairs
	B07[Br-Si]		2D Atom Pairs
	B07[Br-X]		2D Atom Pairs
	B07[I-I]	. •	2D Atom Pairs
3765	B07[I-B]	Presence/absence of I - B at topological distance 7	2D Atom Pairs
3766	B07[I-Si]	Presence/absence of I - Si at topological distance 7	2D Atom Pairs
	B07[I-X]		2D Atom Pairs
	B07[B-B]		2D Atom Pairs
		, ,	2D Atom Pairs
	B07[B-Si]		
	B07[B-X]		2D Atom Pairs
	B07[Si-Si]	Presence/absence of Si - Si at topological distance 7	2D Atom Pairs
3772	B07[Si-X]	Presence/absence of Si - X at topological distance 7	2D Atom Pairs
	B07[X-X]		2D Atom Pairs
	B08[C-C]	. •	2D Atom Pairs
	B08[C-N]	. •	2D Atom Pairs
	B08[C-O]		2D Atom Pairs
3777	B08[C-S]	Presence/absence of C - S at topological distance 8	2D Atom Pairs
3778	B08[C-P]	Presence/absence of C - P at topological distance 8	2D Atom Pairs
	B08[C-F]		2D Atom Pairs
	B08[C-CI]	, ,	2D Atom Pairs
3781	B08[C-Br]	. •	2D Atom Pairs
3782	B08[C-I]	Presence/absence of C - I at topological distance 8	2D Atom Pairs
3783	B08[C-B]	Presence/absence of C - B at topological distance 8	2D Atom Pairs
3784	B08[C-Si]	Presence/absence of C - Si at topological distance 8	2D Atom Pairs
	B08[C-X]		2D Atom Pairs
	B08[N-N]		2D Atom Pairs
	B08[N-O]		2D Atom Pairs
3788	B08[N-S]		2D Atom Pairs
3789	B08[N-P]	Presence/absence of N - P at topological distance 8	2D Atom Pairs
3790	B08[N-F]	Presence/absence of N - F at topological distance 8	2D Atom Pairs
	B08[N-CI]	. •	2D Atom Pairs
	B08[N-Br]	. •	2D Atom Pairs
	B08[N-I]	, ,	2D Atom Pairs
3794	B08[N-B]	Presence/absence of N - B at topological distance 8	2D Atom Pairs
3795	B08[N-Si]	Presence/absence of N - Si at topological distance 8	2D Atom Pairs
	B08[N-X]		2D Atom Pairs
	B08[O-O]		2D Atom Pairs
		·	
	B08[O-S]	, ,	2D Atom Pairs
3799	B08[O-P]	Presence/absence of O - P at topological distance 8	2D Atom Pairs
3800	B08[O-F]	Presence/absence of O - F at topological distance 8	2D Atom Pairs
3801	B08[O-CI]	Presence/absence of O - CI at topological distance 8	2D Atom Pairs
	B08[O-Br]		2D Atom Pairs
	B08[O-I]		
			2D Atom Pairs
	B08[O-B]		2D Atom Pairs
	B08[O-Si]		2D Atom Pairs
3806	B08[O-X]	Presence/absence of O - X at topological distance 8	2D Atom Pairs
	B08[S-S]		2D Atom Pairs
	B08[S-P]		2D Atom Pairs
	B08[S-F]		2D Atom Pairs
		, ,	
	B08[S-CI]		2D Atom Pairs
	B08[S-Br]	, ,	2D Atom Pairs
3812	B08[S-I]	Presence/absence of S - I at topological distance 8	2D Atom Pairs
	B08[S-B]		2D Atom Pairs
	B08[S-Si]		2D Atom Pairs
			2D Atom Pairs
	B08[S-X]		
	B08[P-P]	······································	2D Atom Pairs
3817	B08[P-F]	Presence/absence of P - F at topological distance 8	2D Atom Pairs
	B08[P-CI]		2D Atom Pairs
	B08[P-Br]		2D Atom Pairs
	B08[P-I]		2D Atom Pairs
	B08[P-B]		2D Atom Pairs
	B08[P-Si]		2D Atom Pairs
3823	B08[P-X]	Presence/absence of P - X at topological distance 8	2D Atom Pairs
	B08[F-F]		2D Atom Pairs
	B08[F-CI]		2D Atom Pairs
	B08[F-Br]		2D Atom Pairs
	B08[F-I]		2D Atom Pairs
3828	B08[F-B]	Presence/absence of F - B at topological distance 8	2D Atom Pairs
	B08[F-Si]		2D Atom Pairs
	B08[F-X]		2D Atom Pairs
			2D Atom Pairs
	B08[CI-CI]		
	B08[CI-Br]		2D Atom Pairs
	B08[CI-I]		2D Atom Pairs
	B08[CI-B]		2D Atom Pairs
3835	B08[CI-Si]	Presence/absence of CI - Si at topological distance 8	2D Atom Pairs
	B08[CI-X]		2D Atom Pairs



3837	B08[Br-Br]	Presence/absence of Br - Br at topological distance 8	2D Atom Pairs
	B08[Br-I]	Presence/absence of Br - I at topological distance 8	2D Atom Pairs
	B08[Br-B]		2D Atom Pairs
	B08[Br-Si]		2D Atom Pairs
	B08[Br-X]		2D Atom Pairs
	B08[I-I]		2D Atom Pairs
	B08[I-B]	Presence/absence of I - B at topological distance 8	2D Atom Pairs
3844	B08[I-Si]	Presence/absence of I - Si at topological distance 8	2D Atom Pairs
	B08[I-X]		2D Atom Pairs
	B08[B-B]		2D Atom Pairs
	B08[B-Si]	· ·	2D Atom Pairs
	B08[B-X]		2D Atom Pairs
3849	B08[Si-Si]	Presence/absence of Si - Si at topological distance 8	2D Atom Pairs
3850	B08[Si-X]	Presence/absence of Si - X at topological distance 8	2D Atom Pairs
3851	B08[X-X]	Presence/absence of X - X at topological distance 8	2D Atom Pairs
	B09[C-C]		2D Atom Pairs
	B09[C-N]		2D Atom Pairs
	B09[C-O]		2D Atom Pairs
3855	B09[C-S]	Presence/absence of C - S at topological distance 9	2D Atom Pairs
3856	B09[C-P]	Presence/absence of C - P at topological distance 9	2D Atom Pairs
3857	B09[C-F]	Presence/absence of C - F at topological distance 9	2D Atom Pairs
	B09[C-CI]		2D Atom Pairs
	B09[C-Br]	, ,	2D Atom Pairs
	B09[C-I]		2D Atom Pairs
3861	B09[C-B]	Presence/absence of C - B at topological distance 9	2D Atom Pairs
3862	B09[C-Si]	Presence/absence of C - Si at topological distance 9	2D Atom Pairs
	B09[C-X]		2D Atom Pairs
	B09[N-N]		2D Atom Pairs
	B09[N-O]	·	2D Atom Pairs
	B09[N-S]	Presence/absence of N - S at topological distance 9	2D Atom Pairs
3867	B09[N-P]	Presence/absence of N - P at topological distance 9	2D Atom Pairs
	B09[N-F]		2D Atom Pairs
			2D Atom Pairs
	B09[N-CI]		
	B09[N-Br]	, ,	2D Atom Pairs
	B09[N-I]		2D Atom Pairs
3872	B09[N-B]	Presence/absence of N - B at topological distance 9	2D Atom Pairs
3873	B09[N-Si]	Presence/absence of N - Si at topological distance 9	2D Atom Pairs
	B09[N-X]		2D Atom Pairs
	B09[O-O]		2D Atom Pairs
3876	B09[O-S]	Presence/absence of O - S at topological distance 9	2D Atom Pairs
3877	B09[O-P]	Presence/absence of O - P at topological distance 9	2D Atom Pairs
	B09[O-F]		2D Atom Pairs
	B09[O-CI]		2D Atom Pairs
	B09[O-Br]		2D Atom Pairs
	B09[O-I]	Presence/absence of O - I at topological distance 9	2D Atom Pairs
3882	B09[O-B]	Presence/absence of O - B at topological distance 9	2D Atom Pairs
	B09[O-Si]		2D Atom Pairs
	B09[O-X]		2D Atom Pairs
	B09[S-S]		2D Atom Pairs
	B09[S-P]	, 0	2D Atom Pairs
3887	B09[S-F]	Presence/absence of S - F at topological distance 9	2D Atom Pairs
3888	B09[S-CI]	Presence/absence of S - Cl at topological distance 9	2D Atom Pairs
	B09[S-Br]		2D Atom Pairs
			2D Atom Pairs
	B09[S-I]	, 0	
	B09[S-B]		2D Atom Pairs
3892	B09[S-Si]	Presence/absence of S - Si at topological distance 9	2D Atom Pairs
3893	B09[S-X]	Presence/absence of S - X at topological distance 9	2D Atom Pairs
3894	B09[P-P]		2D Atom Pairs
	B09[P-F]	, 0	2D Atom Pairs
	B09[P-CI]		2D Atom Pairs
	B09[P-Br]		2D Atom Pairs
	B09[P-I]		2D Atom Pairs
3899	B09[P-B]	Presence/absence of P - B at topological distance 9	2D Atom Pairs
	B09[P-Si]		2D Atom Pairs
	B09[P-X]		2D Atom Pairs
	B09[F-K]		
		, ,	2D Atom Pairs
	B09[F-CI]		2D Atom Pairs
	B09[F-Br]		2D Atom Pairs
3905	B09[F-I]	Presence/absence of F - I at topological distance 9	2D Atom Pairs
	B09[F-B]		2D Atom Pairs
	B09[F-Si]		2D Atom Pairs
	B09[F-X]		2D Atom Pairs
	B09[CI-CI]		2D Atom Pairs
3910	B09[CI-Br]		2D Atom Pairs
3911	B09[CI-I]		2D Atom Pairs
	B09[CI-B]		2D Atom Pairs
	B09[CI-Si]		2D Atom Pairs
	B09[CI-X]		2D Atom Pairs
	B09[Br-Br]		2D Atom Pairs
3916	B09[Br-I]	Presence/absence of Br - I at topological distance 9	2D Atom Pairs
3917	B09[Br-B]	Presence/absence of Br - B at topological distance 9	2D Atom Pairs
	B09[Br-Si]		2D Atom Pairs
	B09[Br-X]		2D Atom Pairs
	B09[I-I]		2D Atom Pairs
3921	B09[I-B]	Presence/absence of I - B at topological distance 9	2D Atom Pairs
	B09[I-Si]		2D Atom Pairs
	B09[I-X]		2D Atom Pairs
	B09[B-B]	, 0	2D Atom Pairs
	B09[B-Si]		2D Atom Pairs
3926	B09[B-X]	Presence/absence of B - X at topological distance 9	2D Atom Pairs
	B09[Si-Si]		2D Atom Pairs
	B09[Si-X]		2D Atom Pairs
	B09[X-X]		2D Atom Pairs
	B10[C-C]		2D Atom Pairs
	B10[C-N]		2D Atom Pairs
	B10[C-O]		2D Atom Pairs
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3933	B10[C-S]	Presence/absence of C - S at topological distance 10	2D Atom Pairs
3934	B10[C-P]	Presence/absence of C - P at topological distance 10	2D Atom Pairs
3935	B10[C-F]	Presence/absence of C - F at topological distance 10	2D Atom Pairs
	B10[C-CI]	Presence/absence of C - Cl at topological distance 10	2D Atom Pairs
	B10[C-Br]	Presence/absence of C - Br at topological distance 10	2D Atom Pairs
	B10[C-I]	Presence/absence of C - I at topological distance 10	2D Atom Pairs
	B10[C-B]	Presence/absence of C - B at topological distance 10	2D Atom Pairs
3940	B10[C-Si]	Presence/absence of C - Si at topological distance 10	2D Atom Pairs
3941	B10[C-X]	Presence/absence of C - X at topological distance 10	2D Atom Pairs
	B10[N-N]	Presence/absence of N - N at topological distance 10	2D Atom Pairs
	B10[N-O]	Presence/absence of N - O at topological distance 10	2D Atom Pairs
	B10[N-S]	Presence/absence of N - S at topological distance 10	2D Atom Pairs
	B10[N-P]	Presence/absence of N - P at topological distance 10	2D Atom Pairs
3946	B10[N-F]	Presence/absence of N - F at topological distance 10	2D Atom Pairs
3947	B10[N-CI]	Presence/absence of N - Cl at topological distance 10	2D Atom Pairs
	B10[N-Br]	Presence/absence of N - Br at topological distance 10	2D Atom Pairs
	B10[N-I]	Presence/absence of N - I at topological distance 10	2D Atom Pairs
		· ·	
	B10[N-B]	Presence/absence of N - B at topological distance 10	2D Atom Pairs
3951	B10[N-Si]	Presence/absence of N - Si at topological distance 10	2D Atom Pairs
3952	B10[N-X]	Presence/absence of N - X at topological distance 10	2D Atom Pairs
3953	B10[O-O]	Presence/absence of O - O at topological distance 10	2D Atom Pairs
	B10[O-S]	Presence/absence of O - S at topological distance 10	2D Atom Pairs
	B10[O-P]	Presence/absence of O - P at topological distance 10	2D Atom Pairs
	B10[O-F]	Presence/absence of O - F at topological distance 10	2D Atom Pairs
3957	B10[O-CI]	Presence/absence of O - Cl at topological distance 10	2D Atom Pairs
3958	B10[O-Br]	Presence/absence of O - Br at topological distance 10	2D Atom Pairs
	B10[O-I]	Presence/absence of O - I at topological distance 10	2D Atom Pairs
	B10[O-B]	Presence/absence of O - B at topological distance 10	2D Atom Pairs
	B10[O-Si]	Presence/absence of O - Si at topological distance 10	2D Atom Pairs
	B10[O-X]	Presence/absence of O - X at topological distance 10	2D Atom Pairs
3963	B10[S-S]	Presence/absence of S - S at topological distance 10	2D Atom Pairs
	B10[S-P]	Presence/absence of S - P at topological distance 10	2D Atom Pairs
	B10[S-F]	Presence/absence of S - F at topological distance 10	2D Atom Pairs
	B10[S-CI]	· ·	
		Presence/absence of S - Cl at topological distance 10	2D Atom Pairs
	B10[S-Br]	Presence/absence of S - Br at topological distance 10	2D Atom Pairs
3968	B10[S-I]	Presence/absence of S - I at topological distance 10	2D Atom Pairs
3969	B10[S-B]	Presence/absence of S - B at topological distance 10	2D Atom Pairs
3970	B10[S-Si]	Presence/absence of S - Si at topological distance 10	2D Atom Pairs
	B10[S-X]	Presence/absence of S - X at topological distance 10	2D Atom Pairs
	B10[P-P]	Presence/absence of P - P at topological distance 10	2D Atom Pairs
	B10[P-F]	Presence/absence of P - F at topological distance 10	2D Atom Pairs
	B10[P-CI]	Presence/absence of P - Cl at topological distance 10	2D Atom Pairs
3975	B10[P-Br]	Presence/absence of P - Br at topological distance 10	2D Atom Pairs
3976	B10[P-I]	Presence/absence of P - I at topological distance 10	2D Atom Pairs
3977	B10[P-B]	Presence/absence of P - B at topological distance 10	2D Atom Pairs
	B10[P-Si]	Presence/absence of P - Si at topological distance 10	2D Atom Pairs
	B10[P-X]	Presence/absence of P - X at topological distance 10	2D Atom Pairs
	B10[F-F]	Presence/absence of F - F at topological distance 10	2D Atom Pairs
	B10[F-CI]	Presence/absence of F - Cl at topological distance 10	2D Atom Pairs
	B10[F-Br]	Presence/absence of F - Br at topological distance 10	2D Atom Pairs
3983	B10[F-I]	Presence/absence of F - I at topological distance 10	2D Atom Pairs
3984	B10[F-B]	Presence/absence of F - B at topological distance 10	2D Atom Pairs
3985	B10[F-Si]	Presence/absence of F - Si at topological distance 10	2D Atom Pairs
	B10[F-X]	Presence/absence of F - X at topological distance 10	2D Atom Pairs
	B10[CI-CI]	Presence/absence of CI - CI at topological distance 10	2D Atom Pairs
			2D Atom Pairs
	B10[CI-Br]	Presence/absence of CI - Br at topological distance 10	
	B10[CI-I]	Presence/absence of CI - I at topological distance 10	2D Atom Pairs
3990	B10[CI-B]	Presence/absence of CI - B at topological distance 10	2D Atom Pairs
3991	B10[CI-Si]	Presence/absence of CI - Si at topological distance 10	2D Atom Pairs
	B10[CI-X]	Presence/absence of CI - X at topological distance 10	2D Atom Pairs
	B10[Br-Br]	Presence/absence of Br - Br at topological distance 10	2D Atom Pairs
			2D Atom Pairs
	B10[Br-I]	Presence/absence of Br - I at topological distance 10	
	B10[Br-B]	Presence/absence of Br - B at topological distance 10	2D Atom Pairs
	B10[Br-Si]	Presence/absence of Br - Si at topological distance 10	2D Atom Pairs
3997	B10[Br-X]	Presence/absence of Br - X at topological distance 10	2D Atom Pairs
3998	B10[I-I]	Presence/absence of I - I at topological distance 10	2D Atom Pairs
	B10[I-B]	Presence/absence of I - B at topological distance 10	2D Atom Pairs
	B10[I-Si]	Presence/absence of I - Si at topological distance 10	2D Atom Pairs
	B10[I-X]	Presence/absence of I - X at topological distance 10	2D Atom Pairs
	B10[B-B]	Presence/absence of B - B at topological distance 10	2D Atom Pairs
	B10[B-Si]	Presence/absence of B - Si at topological distance 10	2D Atom Pairs
	B10[B-X]	Presence/absence of B - X at topological distance 10	2D Atom Pairs
	B10[Si-Si]	Presence/absence of Si - Si at topological distance 10	2D Atom Pairs
4006	B10[Si-X]	Presence/absence of Si - X at topological distance 10	2D Atom Pairs
	B10[X-X]	Presence/absence of X - X at topological distance 10	2D Atom Pairs
	F01[C-C]	Frequency of C - C at topological distance 1	2D Atom Pairs
	F01[C-N]	Frequency of C - N at topological distance 1	2D Atom Pairs
			2D Atom Pairs
	F01[C-O]	Frequency of C - O at topological distance 1	
	F01[C-S]	Frequency of C - S at topological distance 1	2D Atom Pairs
	F01[C-P]	Frequency of C - P at topological distance 1	2D Atom Pairs
4013	F01[C-F]	Frequency of C - F at topological distance 1	2D Atom Pairs
	F01[C-CI]	Frequency of C - Cl at topological distance 1	2D Atom Pairs
	F01[C-Br]	Frequency of C - Br at topological distance 1	2D Atom Pairs
	F01[C-I]	Frequency of C - I at topological distance 1	2D Atom Pairs
	F01[C-B]	Frequency of C - B at topological distance 1	2D Atom Pairs
	F01[C-Si]	Frequency of C - Si at topological distance 1	2D Atom Pairs
	F01[C-X]	Frequency of C - X at topological distance 1	2D Atom Pairs
4020	F01[N-N]	Frequency of N - N at topological distance 1	2D Atom Pairs
	F01[N-O]	Frequency of N - O at topological distance 1	2D Atom Pairs
	F01[N-S]	Frequency of N - S at topological distance 1	2D Atom Pairs
	F01[N-P]	Frequency of N - P at topological distance 1	2D Atom Pairs
	F01[N-F]	Frequency of N - F at topological distance 1	2D Atom Pairs
	F01[N-CI]	Frequency of N - Cl at topological distance 1	2D Atom Pairs
	F01[N-Br]	Frequency of N - Br at topological distance 1	2D Atom Pairs
4027	F01[N-I]	Frequency of N - I at topological distance 1	2D Atom Pairs
4028	F01[N-B]	Frequency of N - B at topological distance 1	2D Atom Pairs

4029 F01[N-Si]	Frequency of N - Si at topological distance 1	2D Atom Pairs
4030 F01[N-X]	Frequency of N - X at topological distance 1	2D Atom Pairs
4031 F01[O-O]	Frequency of O - O at topological distance 1	2D Atom Pairs
4032 F01[O-S]	Frequency of O - S at topological distance 1	2D Atom Pairs
4033 F01[O-P]	Frequency of O - P at topological distance 1	2D Atom Pairs
4034 F01[O-F]	Frequency of O - F at topological distance 1	2D Atom Pairs
4035 F01[O-CI]	Frequency of O - Cl at topological distance 1	2D Atom Pairs
4036 F01[O-Br]	Frequency of O - Br at topological distance 1	2D Atom Pairs
4037 F01[O-I]	Frequency of O - I at topological distance 1	2D Atom Pairs
4038 F01[O-B]	Frequency of O - B at topological distance 1	2D Atom Pairs
4039 F01[O-Si]	Frequency of O - Si at topological distance 1	2D Atom Pairs
4040 F01[O-X]	Frequency of O - X at topological distance 1	2D Atom Pairs
	Frequency of S - S at topological distance 1	2D Atom Pairs
4041 F01[S-S] 4042 F01[S-P]	Frequency of S - P at topological distance 1	2D Atom Pairs
		2D Atom Pairs
4043 F01[S-F]	Frequency of S - F at topological distance 1 Frequency of S - Cl at topological distance 1	2D Atom Pairs
4044 F01[S-CI]	Frequency of S - Br at topological distance 1	
4045 F01[S-Br]		2D Atom Pairs
4046 F01[S-I]	Frequency of S - I at topological distance 1	2D Atom Pairs
4047 F01[S-B]	Frequency of S - B at topological distance 1	2D Atom Pairs
4048 F01[S-Si]	Frequency of S - Si at topological distance 1	2D Atom Pairs
4049 F01[S-X]	Frequency of S - X at topological distance 1	2D Atom Pairs
4050 F01[P-P]	Frequency of P - P at topological distance 1	2D Atom Pairs
4051 F01[P-F]	Frequency of P - F at topological distance 1	2D Atom Pairs
4052 F01[P-CI]	Frequency of P - Cl at topological distance 1	2D Atom Pairs
4053 F01[P-Br]	Frequency of P - Br at topological distance 1	2D Atom Pairs
4054 F01[P-I]	Frequency of P - I at topological distance 1	2D Atom Pairs
4055 F01[P-B]	Frequency of P - B at topological distance 1	2D Atom Pairs
4056 F01[P-Si]	Frequency of P - Si at topological distance 1	2D Atom Pairs
4057 F01[P-X]	Frequency of P - X at topological distance 1	2D Atom Pairs
4058 F01[F-F]	Frequency of F - F at topological distance 1	2D Atom Pairs
4059 F01[F-CI]	Frequency of F - Cl at topological distance 1	2D Atom Pairs
4060 F01[F-Br]	Frequency of F - Br at topological distance 1	2D Atom Pairs
4061 F01[F-I]	Frequency of F - I at topological distance 1	2D Atom Pairs
		2D Atom Pairs
4062 F01[F-B]	Frequency of F - B at topological distance 1	2D Atom Pairs
4063 F01[F-Si]	Frequency of F - Si at topological distance 1	
4064 F01[F-X]	Frequency of F - X at topological distance 1	2D Atom Pairs
4065 F01[CI-CI]	Frequency of CI - CI at topological distance 1	2D Atom Pairs
4066 F01[CI-Br]	Frequency of CI - Br at topological distance 1	2D Atom Pairs
4067 F01[CI-I]	Frequency of CI - I at topological distance 1	2D Atom Pairs
4068 F01[CI-B]	Frequency of CI - B at topological distance 1	2D Atom Pairs
4069 F01[CI-Si]	Frequency of CI - Si at topological distance 1	2D Atom Pairs
4070 F01[CI-X]	Frequency of CI - X at topological distance 1	2D Atom Pairs
4071 F01[Br-Br]	Frequency of Br - Br at topological distance 1	2D Atom Pairs
4072 F01[Br-I]	Frequency of Br - I at topological distance 1	2D Atom Pairs
4073 F01[Br-B]	Frequency of Br - B at topological distance 1	2D Atom Pairs
4074 F01[Br-Si]	Frequency of Br - Si at topological distance 1	2D Atom Pairs
4075 F01[Br-X]	Frequency of Br - X at topological distance 1	2D Atom Pairs
4076 F01[I-I]	Frequency of I - I at topological distance 1	2D Atom Pairs
4077 F01[I-B]	Frequency of I - B at topological distance 1	2D Atom Pairs
4078 F01[I-Si]	Frequency of I - Si at topological distance 1	2D Atom Pairs
4079 F01[I-X]	Frequency of I - X at topological distance 1	2D Atom Pairs
4080 F01[B-B]	Frequency of B - B at topological distance 1	2D Atom Pairs
4081 F01[B-Si]	Frequency of B - Si at topological distance 1	2D Atom Pairs
4082 F01[B-X]	Frequency of B - X at topological distance 1	2D Atom Pairs
4083 F01[Si-Si]	Frequency of Si - Si at topological distance 1	2D Atom Pairs
4084 F01[Si-X]	Frequency of Si - X at topological distance 1	2D Atom Pairs
4085 F01[X-X]	Frequency of X - X at topological distance 1	2D Atom Pairs
4086 F02[C-C]	Frequency of C - C at topological distance 2	2D Atom Pairs
4087 F02[C-N]	Frequency of C - N at topological distance 2	2D Atom Pairs
4088 F02[C-O]	Frequency of C - O at topological distance 2	2D Atom Pairs
4089 F02[C-S]	Frequency of C - S at topological distance 2	2D Atom Pairs
4090 F02[C-P]	Frequency of C - P at topological distance 2	2D Atom Pairs
4091 F02[C-F]	Frequency of C - F at topological distance 2	2D Atom Pairs
4092 F02[C-CI]	Frequency of C - Cl at topological distance 2	2D Atom Pairs
4093 F02[C-Br]	Frequency of C - Br at topological distance 2	2D Atom Pairs
		2D Atom Pairs
4094 F02[C-I]	Frequency of C - I at topological distance 2 Frequency of C - B at topological distance 2	2D Atom Pairs
4095 F02[C-B] 4096 F02[C-Si]	Frequency of C - Si at topological distance 2	2D Atom Pairs
		2D Atom Pairs
4097 F02[C-X]	Frequency of N. N. at topological distance 2	
4098 F02[N-N]	Frequency of N - N at topological distance 2	2D Atom Pairs
4099 F02[N-O]	Frequency of N - O at topological distance 2	2D Atom Pairs
4100 F02[N-S]	Frequency of N - S at topological distance 2	2D Atom Pairs
4101 F02[N-P]	Frequency of N - P at topological distance 2	2D Atom Pairs
4102 F02[N-F]	Frequency of N - F at topological distance 2	2D Atom Pairs
4103 F02[N-CI]	Frequency of N - Cl at topological distance 2	2D Atom Pairs
4104 F02[N-Br]	Frequency of N - Br at topological distance 2	2D Atom Pairs
4105 F02[N-I]	Frequency of N - I at topological distance 2	2D Atom Pairs
4106 F02[N-B]	Frequency of N - B at topological distance 2	2D Atom Pairs
4107 F02[N-Si]	Frequency of N - Si at topological distance 2	2D Atom Pairs
4108 F02[N-X]	Frequency of N - X at topological distance 2	2D Atom Pairs
4109 F02[O-O]	Frequency of O - O at topological distance 2	2D Atom Pairs
4110 F02[O-S]	Frequency of O - S at topological distance 2	2D Atom Pairs
4111 F02[O-P]	Frequency of O - P at topological distance 2	2D Atom Pairs
4112 F02[O-F]	Frequency of O - F at topological distance 2	2D Atom Pairs
4113 F02[O-Cl]	Frequency of O - Cl at topological distance 2	2D Atom Pairs
4114 F02[O-Br]	Frequency of O - Br at topological distance 2	2D Atom Pairs
4115 F02[O-I]	Frequency of O - I at topological distance 2	2D Atom Pairs
4116 F02[O-B]	Frequency of O - B at topological distance 2	2D Atom Pairs
4117 F02[O-Si]	Frequency of O - Si at topological distance 2	2D Atom Pairs
4118 F02[O-X]	Frequency of O - X at topological distance 2	2D Atom Pairs
4119 F02[S-S]	Frequency of S - S at topological distance 2	2D Atom Pairs
4120 F02[S-P]	Frequency of S - P at topological distance 2	2D Atom Pairs
4121 F02[S-F]	Frequency of S - F at topological distance 2	2D Atom Pairs
4121 F02[S-F] 4122 F02[S-CI]	Frequency of S - P at topological distance 2 Frequency of S - Cl at topological distance 2	2D Atom Pairs
4122 F02[S-GI] 4123 F02[S-Br]	Frequency of S - Criat topological distance 2 Frequency of S - Br at topological distance 2	2D Atom Pairs 2D Atom Pairs
4124 F02[S-I]	Frequency of S - I at topological distance 2 Frequency of S - I at topological distance 2	2D Atom Pairs

4125 F02[S-B]	Frequency of S - B at topological distance 2	2D Atom Pairs
4126 F02[S-Si]	Frequency of S - Si at topological distance 2	2D Atom Pairs
4127 F02[S-X]	Frequency of S - X at topological distance 2	2D Atom Pairs
4128 F02[P-P]	Frequency of P - P at topological distance 2	2D Atom Pairs
4129 F02[P-F]	Frequency of P - F at topological distance 2	2D Atom Pairs
4130 F02[P-CI]	Frequency of P - Cl at topological distance 2	2D Atom Pairs
4131 F02[P-Br]	Frequency of P - Br at topological distance 2	2D Atom Pairs
4132 F02[P-I]	Frequency of P - I at topological distance 2	2D Atom Pairs
4133 F02[P-B]	Frequency of P - B at topological distance 2	2D Atom Pairs
	Frequency of P - Si at topological distance 2	2D Atom Pairs
4134 F02[P-Si]		
4135 F02[P-X]	Frequency of P - X at topological distance 2	2D Atom Pairs
4136 F02[F-F]	Frequency of F - F at topological distance 2	2D Atom Pairs
4137 F02[F-CI]	Frequency of F - CI at topological distance 2	2D Atom Pairs
4138 F02[F-Br]	Frequency of F - Br at topological distance 2	2D Atom Pairs
4139 F02[F-I]	Frequency of F - I at topological distance 2	2D Atom Pairs
4140 F02[F-B]	Frequency of F - B at topological distance 2	2D Atom Pairs
4141 F02[F-Si]	Frequency of F - Si at topological distance 2	2D Atom Pairs
• •		
4142 F02[F-X]	Frequency of F - X at topological distance 2	2D Atom Pairs
4143 F02[CI-CI]	Frequency of CI - CI at topological distance 2	2D Atom Pairs
4144 F02[CI-Br]	Frequency of Cl - Br at topological distance 2	2D Atom Pairs
4145 F02[CI-I]	Frequency of Cl - I at topological distance 2	2D Atom Pairs
4146 F02[CI-B]	Frequency of CI - B at topological distance 2	2D Atom Pairs
4147 F02[CI-Si]	Frequency of CI - Si at topological distance 2	2D Atom Pairs
		2D Atom Pairs
4148 F02[CI-X]	Frequency of CI - X at topological distance 2	
4149 F02[Br-Br]	Frequency of Br - Br at topological distance 2	2D Atom Pairs
4150 F02[Br-I]	Frequency of Br - I at topological distance 2	2D Atom Pairs
4151 F02[Br-B]	Frequency of Br - B at topological distance 2	2D Atom Pairs
4152 F02[Br-Si]	Frequency of Br - Si at topological distance 2	2D Atom Pairs
4153 F02[Br-X]	Frequency of Br - X at topological distance 2	2D Atom Pairs
4154 F02[I-I]	Frequency of I - I at topological distance 2	2D Atom Pairs
• •	Frequency of I - B at topological distance 2	2D Atom Pairs
4155 F02[I-B]		
4156 F02[I-Si]	Frequency of I - Si at topological distance 2	2D Atom Pairs
4157 F02[I-X]	Frequency of I - X at topological distance 2	2D Atom Pairs
4158 F02[B-B]	Frequency of B - B at topological distance 2	2D Atom Pairs
4159 F02[B-Si]	Frequency of B - Si at topological distance 2	2D Atom Pairs
4160 F02[B-X]	Frequency of B - X at topological distance 2	2D Atom Pairs
4161 F02[Si-Si]	Frequency of Si - Si at topological distance 2	2D Atom Pairs
4162 F02[Si-X]	Frequency of Si - X at topological distance 2	2D Atom Pairs
4163 F02[X-X]	Frequency of X - X at topological distance 2	2D Atom Pairs
4164 F03[C-C]	Frequency of C - C at topological distance 3	2D Atom Pairs
4165 F03[C-N]	Frequency of C - N at topological distance 3	2D Atom Pairs
4166 F03[C-O]	Frequency of C - O at topological distance 3	2D Atom Pairs
4167 F03[C-S]	Frequency of C - S at topological distance 3	2D Atom Pairs
4168 F03[C-P]	Frequency of C - P at topological distance 3	2D Atom Pairs
4169 F03[C-F]	Frequency of C - F at topological distance 3	2D Atom Pairs
4170 F03[C-CI]	Frequency of C - Cl at topological distance 3	2D Atom Pairs
4171 F03[C-Br]	Frequency of C - Br at topological distance 3	2D Atom Pairs
4172 F03[C-I]	Frequency of C - I at topological distance 3	2D Atom Pairs
4173 F03[C-B]	Frequency of C - B at topological distance 3	2D Atom Pairs
4174 F03[C-Si]	Frequency of C - Si at topological distance 3	2D Atom Pairs
4175 F03[C-X]	Frequency of C - X at topological distance 3	2D Atom Pairs
4176 F03[N-N]	Frequency of N - N at topological distance 3	2D Atom Pairs
4177 F03[N-O]	Frequency of N - O at topological distance 3	2D Atom Pairs
4178 F03[N-S]	Frequency of N - S at topological distance 3	2D Atom Pairs
4179 F03[N-P]	Frequency of N - P at topological distance 3	2D Atom Pairs
4180 F03[N-F]	Frequency of N - F at topological distance 3	2D Atom Pairs
4181 F03[N-CI]	Frequency of N - Cl at topological distance 3	2D Atom Pairs
4182 F03[N-Br]	Frequency of N - Br at topological distance 3	2D Atom Pairs
4183 F03[N-I]	Frequency of N - I at topological distance 3	2D Atom Pairs
4184 F03[N-B]	Frequency of N - B at topological distance 3	2D Atom Pairs
4185 F03[N-Si]	Frequency of N - Si at topological distance 3	2D Atom Pairs
4186 F03[N-X]	Frequency of N - X at topological distance 3	2D Atom Pairs
4187 F03[O-O]	Frequency of O - O at topological distance 3	2D Atom Pairs
4188 F03[O-S]	Frequency of O - S at topological distance 3	2D Atom Pairs
4189 F03[O-P]	Frequency of O - 9 at topological distance 3	2D Atom Pairs
4190 F03[O-F]	Frequency of O - F at topological distance 3	2D Atom Pairs
4191 F03[O-CI]	Frequency of O - Cl at topological distance 3	2D Atom Pairs
4192 F03[O-Br]	Frequency of O - Br at topological distance 3	2D Atom Pairs
4193 F03[O-I]	Frequency of O - I at topological distance 3	2D Atom Pairs
4194 F03[O-B]	Frequency of O - B at topological distance 3	2D Atom Pairs
4195 F03[O-Si]	Frequency of O - Si at topological distance 3	2D Atom Pairs
4196 F03[O-X]	Frequency of O - X at topological distance 3	2D Atom Pairs
	Frequency of S - S at topological distance 3 Frequency of S - S at topological distance 3	2D Atom Pairs
4197 F03[S-S]		
4198 F03[S-P]	Frequency of S - P at topological distance 3	2D Atom Pairs
4199 F03[S-F]	Frequency of S - F at topological distance 3	2D Atom Pairs
4200 F03[S-CI]	Frequency of S - CI at topological distance 3	2D Atom Pairs
4201 F03[S-Br]	Frequency of S - Br at topological distance 3	2D Atom Pairs
4202 F03[S-I]	Frequency of S - I at topological distance 3	2D Atom Pairs
4203 F03[S-B]	Frequency of S - B at topological distance 3	2D Atom Pairs
4204 F03[S-Si]	Frequency of S - Si at topological distance 3	2D Atom Pairs
4205 F03[S-X]	Frequency of S - X at topological distance 3	2D Atom Pairs
4206 F03[P-P]	Frequency of P - P at topological distance 3	2D Atom Pairs
4207 F03[P-F]	Frequency of P - F at topological distance 3	2D Atom Pairs
4208 F03[P-CI]	Frequency of P - Cl at topological distance 3	2D Atom Pairs
4209 F03[P-Br]	Frequency of P - Br at topological distance 3	2D Atom Pairs
4210 F03[P-I]	Frequency of P - I at topological distance 3	2D Atom Pairs
4211 F03[P-B]	Frequency of P - B at topological distance 3	2D Atom Pairs
4212 F03[P-Si]	Frequency of P - Si at topological distance 3	2D Atom Pairs
4213 F03[P-X]	Frequency of P - X at topological distance 3	2D Atom Pairs
4214 F03[F-F]	Frequency of F - F at topological distance 3	2D Atom Pairs
4215 F03[F-CI]	Frequency of F - Cl at topological distance 3	2D Atom Pairs
4216 F03[F-Br]	Frequency of F - Br at topological distance 3	2D Atom Pairs
4217 F03[F-II]	Frequency of F - I at topological distance 3	2D Atom Pairs
4218 F03[F-B]	Frequency of F - B at topological distance 3	2D Atom Pairs
4219 F03[F-Si]	Frequency of F - Si at topological distance 3	2D Atom Pairs
4220 F03[F-X]	Frequency of F - X at topological distance 3	2D Atom Pairs

4221	F03[CI-CI]	Frequency of CI - CI at topological distance 3	2D Ato	m Pairs
4222	F03[CI-Br]	Frequency of CI - Br at topological distance 3	2D Ato	m Pairs
4223	F03[CI-I]	Frequency of CI - I at topological distance 3	2D Ato	m Pairs
	F03[CI-B]	Frequency of CI - B at topological distance 3		m Pairs
	F03[CI-Si]	Frequency of CI - Si at topological distance 3		m Pairs
	F03[CI-X]	Frequency of CI - X at topological distance 3		m Pairs
	F03[Br-Br]	Frequency of Br - Br at topological distance 3		m Pairs
	F03[Br-I]	Frequency of Br - I at topological distance 3		m Pairs
4229	F03[Br-B]	Frequency of Br - B at topological distance 3	2D Ato	m Pairs
4230	F03[Br-Si]	Frequency of Br - Si at topological distance 3	2D Ato	m Pairs
4231	F03[Br-X]	Frequency of Br - X at topological distance 3	2D Ato	m Pairs
	F03[I-I]	Frequency of I - I at topological distance 3		m Pairs
	F03[I-B]	Frequency of I - B at topological distance 3		m Pairs
	F03[I-Si]	Frequency of I - Si at topological distance 3		m Pairs
4235	F03[I-X]	Frequency of I - X at topological distance 3	2D Ato	m Pairs
4236	F03[B-B]	Frequency of B - B at topological distance 3	2D Ato	m Pairs
4237	F03[B-Si]	Frequency of B - Si at topological distance 3	2D Ato	m Pairs
4238	F03[B-X]	Frequency of B - X at topological distance 3	2D Ato	m Pairs
	F03[Si-Si]	Frequency of Si - Si at topological distance 3	2D Atc	m Pairs
	F03[Si-X]	Frequency of Si - X at topological distance 3		m Pairs
				m Pairs
	F03[X-X]	Frequency of X - X at topological distance 3		
	F04[C-C]	Frequency of C - C at topological distance 4		m Pairs
4243	F04[C-N]	Frequency of C - N at topological distance 4	2D Ato	m Pairs
4244	F04[C-O]	Frequency of C - O at topological distance 4	2D Ato	m Pairs
4245	F04[C-S]	Frequency of C - S at topological distance 4	2D Ato	m Pairs
	F04[C-P]	Frequency of C - P at topological distance 4		m Pairs
	F04[C-F]	Frequency of C - F at topological distance 4		m Pairs
	F04[C-CI]	Frequency of C - CI at topological distance 4		m Pairs
	F04[C-Br]	Frequency of C - Br at topological distance 4		m Pairs
	F04[C-I]	Frequency of C - I at topological distance 4		m Pairs
	F04[C-B]	Frequency of C - B at topological distance 4		m Pairs
4252	F04[C-Si]	Frequency of C - Si at topological distance 4	2D Ato	m Pairs
	F04[C-X]	Frequency of C - X at topological distance 4		m Pairs
	F04[N-N]	Frequency of N - N at topological distance 4		m Pairs
	F04[N-O]	Frequency of N - O at topological distance 4		m Pairs
		. ,		
	F04[N-S]	Frequency of N - S at topological distance 4		m Pairs
	F04[N-P]	Frequency of N - P at topological distance 4		m Pairs
4258	F04[N-F]	Frequency of N - F at topological distance 4		m Pairs
4259	F04[N-CI]	Frequency of N - Cl at topological distance 4	2D Atc	m Pairs
4260	F04[N-Br]	Frequency of N - Br at topological distance 4	2D Ato	m Pairs
	F04[N-I]	Frequency of N - I at topological distance 4	2D Ato	m Pairs
	F04[N-B]	Frequency of N - B at topological distance 4		m Pairs
	F04[N-Si]	Frequency of N - Si at topological distance 4		m Pairs
	F04[N-X]	Frequency of N - X at topological distance 4		m Pairs
	F04[O-O]	Frequency of O - O at topological distance 4		m Pairs
4266	F04[O-S]	Frequency of O - S at topological distance 4	2D Ato	m Pairs
4267	F04[O-P]	Frequency of O - P at topological distance 4	2D Ato	m Pairs
4268	F04[O-F]	Frequency of O - F at topological distance 4	2D Ato	m Pairs
	F04[O-CI]	Frequency of O - Cl at topological distance 4	2D Ato	m Pairs
	F04[O-Br]	Frequency of O - Br at topological distance 4		m Pairs
				m Pairs
	F04[O-I]	Frequency of O - I at topological distance 4		
	F04[O-B]	Frequency of O - B at topological distance 4		m Pairs
	F04[O-Si]	Frequency of O - Si at topological distance 4		m Pairs
4274	F04[O-X]	Frequency of O - X at topological distance 4	2D Ato	m Pairs
4275	F04[S-S]	Frequency of S - S at topological distance 4	2D Ato	m Pairs
4276	F04[S-P]	Frequency of S - P at topological distance 4	2D Ato	m Pairs
	F04[S-F]	Frequency of S - F at topological distance 4		m Pairs
	F04[S-CI]	Frequency of S - Cl at topological distance 4		m Pairs
		Frequency of S - Br at topological distance 4		m Pairs
	F04[S-Br]			
	F04[S-I]	Frequency of S - I at topological distance 4		m Pairs
	F04[S-B]	Frequency of S - B at topological distance 4		m Pairs
4282	F04[S-Si]	Frequency of S - Si at topological distance 4	2D Ato	m Pairs
4283	F04[S-X]	Frequency of S - X at topological distance 4	2D Ato	m Pairs
4284	F04[P-P]	Frequency of P - P at topological distance 4	2D Ato	m Pairs
	F04[P-F]	Frequency of P - F at topological distance 4		m Pairs
	F04[P-CI]	Frequency of P - Cl at topological distance 4		m Pairs
	F04[P-Br]	Frequency of P - Br at topological distance 4		m Pairs
		Frequency of P - I at topological distance 4		m Pairs
	F04[P-I]			
	F04[P-B]	Frequency of P - B at topological distance 4		m Pairs
	F04[P-Si]	Frequency of P - Si at topological distance 4		m Pairs
	F04[P-X]	Frequency of P - X at topological distance 4		m Pairs
	F04[F-F]	Frequency of F - F at topological distance 4	2D Ato	m Pairs
4293	F04[F-CI]	Frequency of F - Cl at topological distance 4	2D Ato	m Pairs
	F04[F-Br]	Frequency of F - Br at topological distance 4		m Pairs
	F04[F-I]	Frequency of F - I at topological distance 4		m Pairs
	F04[F-B]	Frequency of F - B at topological distance 4		m Pairs
				om Pairs
	F04[F-Si]	Frequency of F - Si at topological distance 4		
	F04[F-X]	Frequency of F - X at topological distance 4		m Pairs
	F04[CI-CI]	Frequency of CI - CI at topological distance 4		m Pairs
4300	F04[CI-Br]	Frequency of CI - Br at topological distance 4	2D Ato	m Pairs
4301	F04[CI-I]	Frequency of CI - I at topological distance 4	2D Ato	m Pairs
	F04[CI-B]	Frequency of CI - B at topological distance 4		m Pairs
	F04[CI-Si]	Frequency of CI - Si at topological distance 4		m Pairs
	F04[CI-X]	Frequency of CI - X at topological distance 4		m Pairs
	F04[Br-Br]	Frequency of Br - Br at topological distance 4		m Pairs
	F04[Br-I]	Frequency of Br - I at topological distance 4		m Pairs
	F04[Br-B]	Frequency of Br - B at topological distance 4		m Pairs
4308	F04[Br-Si]	Frequency of Br - Si at topological distance 4	2D Ato	m Pairs
	F04[Br-X]	Frequency of Br - X at topological distance 4	2D Ato	m Pairs
	F04[I-I]	Frequency of I - I at topological distance 4		m Pairs
	F04[I-B]	Frequency of I - B at topological distance 4		m Pairs
	F04[I-Si]	Frequency of I - Si at topological distance 4		m Pairs
	F04[I-X]	Frequency of I - X at topological distance 4		m Pairs
	F04[B-B]	Frequency of B - B at topological distance 4		m Pairs
	F04[B-Si]	Frequency of B - Si at topological distance 4		m Pairs
4316	F04[B-X]	Frequency of B - X at topological distance 4	2D Ato	m Pairs

	F04[Si-Si]		2D Atom Pairs
4318	F04[Si-X]	Frequency of Si - X at topological distance 4	2D Atom Pairs
4319	F04[X-X]	Frequency of X - X at topological distance 4	2D Atom Pairs
4320	F05[C-C]	Frequency of C - C at topological distance 5	2D Atom Pairs
	F05[C-N]	. ,	2D Atom Pairs
	F05[C-O]		2D Atom Pairs
	F05[C-S]		2D Atom Pairs
	F05[C-P]		
			2D Atom Pairs
	F05[C-F]	, ,	2D Atom Pairs
	F05[C-CI]		2D Atom Pairs
4327	F05[C-Br]	Frequency of C - Br at topological distance 5	2D Atom Pairs
4328	F05[C-I]	Frequency of C - I at topological distance 5	2D Atom Pairs
	F05[C-B]		2D Atom Pairs
	F05[C-Si]		2D Atom Pairs
	F05[C-X]		2D Atom Pairs
	F05[N-N]		2D Atom Pairs
4333	F05[N-O]	Frequency of N - O at topological distance 5	2D Atom Pairs
4334	F05[N-S]		2D Atom Pairs
4335	F05[N-P]	Frequency of N - P at topological distance 5	2D Atom Pairs
4336	F05[N-F]		2D Atom Pairs
	F05[N-CI]		2D Atom Pairs
	F05[N-Br]		2D Atom Pairs
	F05[N-I]	. ,	2D Atom Pairs
	F05[N-B]	. ,	2D Atom Pairs
	F05[N-Si]		2D Atom Pairs
4342	F05[N-X]	Frequency of N - X at topological distance 5	2D Atom Pairs
4343	F05[O-O]	Frequency of O - O at topological distance 5	2D Atom Pairs
	F05[O-S]		2D Atom Pairs
	F05[O-P]		2D Atom Pairs
	F05[O-F]		2D Atom Pairs
	F05[O-CI]	, , , , ,	2D Atom Pairs
		. ,	
	F05[O-Br]		2D Atom Pairs
	F05[O-I]		2D Atom Pairs
	F05[O-B]	- 1 3	2D Atom Pairs
4351	F05[O-Si]	Frequency of O - Si at topological distance 5	2D Atom Pairs
4352	F05[O-X]	Frequency of O - X at topological distance 5	2D Atom Pairs
	F05[S-S]		2D Atom Pairs
	F05[S-P]	. ,	2D Atom Pairs
	F05[S-F]		2D Atom Pairs
	F05[S-CI]	. ,	2D Atom Pairs
	F05[S-Br]	, , , , ,	2D Atom Pairs
4358	F05[S-I]	Frequency of S - I at topological distance 5	2D Atom Pairs
4359	F05[S-B]	Frequency of S - B at topological distance 5	2D Atom Pairs
4360	F05[S-Si]	Frequency of S - Si at topological distance 5	2D Atom Pairs
	F05[S-X]		2D Atom Pairs
	F05[P-P]		2D Atom Pairs
	F05[P-F]		2D Atom Pairs
	F05[P-CI]	. ,	2D Atom Pairs
	F05[P-Br]	. ,	2D Atom Pairs
4366	F05[P-I]	Frequency of P - I at topological distance 5	2D Atom Pairs
4367	F05[P-B]	Frequency of P - B at topological distance 5	2D Atom Pairs
4368	F05[P-Si]	Frequency of P - Si at topological distance 5	2D Atom Pairs
	F05[P-X]		2D Atom Pairs
	F05[F-F]	. ,	2D Atom Pairs
	F05[F-CI]		2D Atom Pairs
	F05[F-Br]	. ,	2D Atom Pairs
	F05[F-I]		2D Atom Pairs
	F05[F-B]	· · ·	2D Atom Pairs
4375	F05[F-Si]	Frequency of F - Si at topological distance 5	2D Atom Pairs
4376	F05[F-X]	Frequency of F - X at topological distance 5	2D Atom Pairs
4377	F05[CI-CI]	Frequency of CI - CI at topological distance 5	2D Atom Pairs
	F05[CI-Br]		2D Atom Pairs
	F05[CI-I]		2D Atom Pairs
	F05[CI-B]		2D Atom Pairs
	F05[CI-B]	- 1 7	
			2D Atom Pairs
	F05[CI-X]	. ,	2D Atom Pairs
	F05[Br-Br]		2D Atom Pairs
	F05[Br-I]		2D Atom Pairs
	F05[Br-B]		2D Atom Pairs
4386	F05[Br-Si]	Frequency of Br - Si at topological distance 5	2D Atom Pairs
	F05[Br-X]	Frequency of Br - X at topological distance 5	2D Atom Pairs
	F05[I-I]		2D Atom Pairs
	F05[I-B]		2D Atom Pairs
	F05[I-Si]		2D Atom Pairs
	F05[I-X]		2D Atom Pairs
	F05[B-B]		2D Atom Pairs
	F05[B-Si]		2D Atom Pairs
	F05[B-X]		2D Atom Pairs
4395	F05[Si-Si]	Frequency of Si - Si at topological distance 5	2D Atom Pairs
	F05[Si-X]		2D Atom Pairs
	F05[X-X]		2D Atom Pairs
	F06[C-C]		2D Atom Pairs
	F06[C-N]		2D Atom Pairs
	F06[C-O]	. ,	2D Atom Pairs
	F06[C-S]		2D Atom Pairs
	F06[C-P]		2D Atom Pairs
4403	F06[C-F]	Frequency of C - F at topological distance 6	2D Atom Pairs
4404	F06[C-CI]	Frequency of C - Cl at topological distance 6	2D Atom Pairs
	F06[C-Br]		2D Atom Pairs
	F06[C-I]		2D Atom Pairs
	F06[C-B]		2D Atom Pairs
	F06[C-Si]		2D Atom Pairs
	F06[C-X]		2D Atom Pairs
	F06[N-N]		2D Atom Pairs
	F06[N-O]		2D Atom Pairs
4412	F06[N-S]	Frequency of N - S at topological distance 6	2D Atom Pairs

4413	F06[N-P]	Frequency of N - P at topological distance 6	2D Atom Pairs
4414	F06[N-F]	Frequency of N - F at topological distance 6	2D Atom Pairs
	F06[N-CI]	Frequency of N - Cl at topological distance 6	2D Atom Pairs
4416	F06[N-Br]	Frequency of N - Br at topological distance 6	2D Atom Pairs
	F06[N-I]	. ,	2D Atom Pairs
	F06[N-B]		2D Atom Pairs
	F06[N-Si]		2D Atom Pairs
	F06[N-X]		2D Atom Pairs
	F06[O-O]	Frequency of O - O at topological distance 6	2D Atom Pairs
	F06[O-S]		2D Atom Pairs
	F06[O-P]		2D Atom Pairs
		· · · ·	
	F06[O-F]		2D Atom Pairs
	F06[O-CI]	Frequency of O - Cl at topological distance 6	2D Atom Pairs
	F06[O-Br]		2D Atom Pairs
	F06[O-I]	. ,	2D Atom Pairs
	F06[O-B]	Frequency of O - B at topological distance 6	2D Atom Pairs
	F06[O-Si]		2D Atom Pairs
	F06[O-X]	Frequency of O - X at topological distance 6	2D Atom Pairs
	F06[S-S]	Frequency of S - S at topological distance 6	2D Atom Pairs
4432	F06[S-P]	Frequency of S - P at topological distance 6	2D Atom Pairs
4433	F06[S-F]	Frequency of S - F at topological distance 6	2D Atom Pairs
4434	F06[S-CI]	Frequency of S - Cl at topological distance 6	2D Atom Pairs
4435	F06[S-Br]	Frequency of S - Br at topological distance 6	2D Atom Pairs
4436	F06[S-I]	Frequency of S - I at topological distance 6	2D Atom Pairs
	F06[S-B]		2D Atom Pairs
	F06[S-Si]		2D Atom Pairs
	F06[S-X]		2D Atom Pairs
	F06[P-P]	Frequency of P - P at topological distance 6	2D Atom Pairs
	F06[P-F]		2D Atom Pairs
		- 1 3	2D Atom Pairs
	F06[P-CI]	. ,	
	F06[P-Br]		2D Atom Pairs
	F06[P-I]	Frequency of P - I at topological distance 6	2D Atom Pairs
	F06[P-B]		2D Atom Pairs
4446	F06[P-Si]	Frequency of P - Si at topological distance 6	2D Atom Pairs
4447	F06[P-X]	Frequency of P - X at topological distance 6	2D Atom Pairs
4448	F06[F-F]	Frequency of F - F at topological distance 6	2D Atom Pairs
4449	F06[F-CI]	Frequency of F - CI at topological distance 6	2D Atom Pairs
	F06[F-Br]		2D Atom Pairs
4451	F06[F-I]		2D Atom Pairs
	F06[F-B]		2D Atom Pairs
	F06[F-Si]	Frequency of F - Si at topological distance 6	2D Atom Pairs
	F06[F-X]	Frequency of F - X at topological distance 6	2D Atom Pairs
	F06[CI-CI]		2D Atom Pairs
	F06[CI-Br]		2D Atom Pairs
	F06[CI-I]	. ,	2D Atom Pairs
	F06[CI-B]		2D Atom Pairs
	F06[CI-Si]	Frequency of CI - Si at topological distance 6	2D Atom Pairs
	F06[CI-X]	. ,	2D Atom Pairs
4461	F06[Br-Br]	Frequency of Br - Br at topological distance 6	2D Atom Pairs
4462	F06[Br-I]	Frequency of Br - I at topological distance 6	2D Atom Pairs
4463	F06[Br-B]	Frequency of Br - B at topological distance 6	2D Atom Pairs
4464	F06[Br-Si]	Frequency of Br - Si at topological distance 6	2D Atom Pairs
	F06[Br-X]		2D Atom Pairs
	F06[I-I]	Frequency of I - I at topological distance 6	2D Atom Pairs
	F06[I-B]		2D Atom Pairs
	F06[I-Si]	· · ·	2D Atom Pairs
	F06[I-X]	. ,	2D Atom Pairs
	F06[B-B]		2D Atom Pairs
	F06[B-Si]	Frequency of B - Si at topological distance 6	2D Atom Pairs
	F06[B-X]	Frequency of B - X at topological distance 6	2D Atom Pairs
	F06[Si-Si]	Frequency of Si - Si at topological distance 6	2D Atom Pairs
	F06[Si-X]		2D Atom Pairs
	F06[X-X]		2D Atom Pairs
	F07[C-C]	- 1 7	2D Atom Pairs
	F07[C-N]		2D Atom Pairs
4478	F07[C-O]	Frequency of C - O at topological distance 7	2D Atom Pairs
	F07[C-S]	. ,	2D Atom Pairs
	F07[C-P]		2D Atom Pairs
	F07[C-F]		2D Atom Pairs
4482	F07[C-CI]	Frequency of C - CI at topological distance 7	2D Atom Pairs
4483	F07[C-Br]	Frequency of C - Br at topological distance 7	2D Atom Pairs
	F07[C-I]	Frequency of C - I at topological distance 7	2D Atom Pairs
	F07[C-B]		2D Atom Pairs
	F07[C-Si]		2D Atom Pairs
	F07[C-X]	Frequency of C - X at topological distance 7	2D Atom Pairs
	F07[N-N]		2D Atom Pairs
	F07[N-O]		2D Atom Pairs
	F07[N-S]		2D Atom Pairs
	F07[N-P]		2D Atom Pairs
	F07[N-F]	. ,	2D Atom Pairs
			2D Atom Pairs
	F07[N-CI]		
	F07[N-Br]		2D Atom Pairs
	F07[N-I]		2D Atom Pairs
	F07[N-B]		2D Atom Pairs
	F07[N-Si]	· · ·	2D Atom Pairs
	F07[N-X]		2D Atom Pairs
	F07[O-O]		2D Atom Pairs
	F07[O-S]		2D Atom Pairs
	F07[O-P]	Frequency of O - P at topological distance 7	2D Atom Pairs
	F07[O-F]	. ,	2D Atom Pairs
4503	F07[O-CI]	Frequency of O - Cl at topological distance 7	2D Atom Pairs
	F07[O-Br]		2D Atom Pairs
	F07[O-I]		2D Atom Pairs
	F07[O-B]	Frequency of O - B at topological distance 7	2D Atom Pairs
	F07[O-Si]	Frequency of O - Si at topological distance 7	2D Atom Pairs
	F07[O-X]	Frequency of O - X at topological distance 7	2D Atom Pairs

	F07[S-S]	Frequency of S - S at topological distance 7	2D Atom Pairs
4510	F07[S-P]	Frequency of S - P at topological distance 7	2D Atom Pairs
4511	F07[S-F]	Frequency of S - F at topological distance 7	2D Atom Pairs
4512	F07[S-CI]	Frequency of S - Cl at topological distance 7	2D Atom Pairs
	F07[S-Br]	Frequency of S - Br at topological distance 7	2D Atom Pairs
	F07[S-I]	Frequency of S - I at topological distance 7	2D Atom Pairs
	F07[S-B]	Frequency of S - B at topological distance 7	2D Atom Pairs
	F07[S-Si]	Frequency of S - Si at topological distance 7	2D Atom Pairs
	F07[S-X]	Frequency of S - X at topological distance 7	2D Atom Pairs
4518	F07[P-P]	Frequency of P - P at topological distance 7	2D Atom Pairs
4519	F07[P-F]	Frequency of P - F at topological distance 7	2D Atom Pairs
4520	F07[P-CI]	Frequency of P - Cl at topological distance 7	2D Atom Pairs
	F07[P-Br]	Frequency of P - Br at topological distance 7	2D Atom Pairs
	F07[P-I]	Frequency of P - I at topological distance 7	2D Atom Pairs
			2D Atom Pairs
	F07[P-B]	Frequency of P - B at topological distance 7	
	F07[P-Si]	Frequency of P - Si at topological distance 7	2D Atom Pairs
	F07[P-X]	Frequency of P - X at topological distance 7	2D Atom Pairs
4526	F07[F-F]	Frequency of F - F at topological distance 7	2D Atom Pairs
4527	F07[F-CI]	Frequency of F - Cl at topological distance 7	2D Atom Pairs
4528	F07[F-Br]	Frequency of F - Br at topological distance 7	2D Atom Pairs
	F07[F-I]	Frequency of F - I at topological distance 7	2D Atom Pairs
	F07[F-B]	Frequency of F - B at topological distance 7	2D Atom Pairs
	F07[F-Si]	Frequency of F - Si at topological distance 7	2D Atom Pairs
	F07[F-X]	Frequency of F - X at topological distance 7	2D Atom Pairs
	F07[CI-CI]	Frequency of CI - CI at topological distance 7	2D Atom Pairs
	F07[CI-Br]	Frequency of CI - Br at topological distance 7	2D Atom Pairs
4535	F07[CI-I]	Frequency of Cl - I at topological distance 7	2D Atom Pairs
4536	F07[CI-B]	Frequency of CI - B at topological distance 7	2D Atom Pairs
	F07[CI-Si]	Frequency of CI - Si at topological distance 7	2D Atom Pairs
	F07[CI-X]	Frequency of CI - X at topological distance 7	2D Atom Pairs
	F07[Br-Br]	Frequency of Br - Br at topological distance 7	2D Atom Pairs
	F07[Br-I]	Frequency of Br - I at topological distance 7	2D Atom Pairs
			2D Atom Pairs
	F07[Br-B]	Frequency of Br - B at topological distance 7	
	F07[Br-Si]	Frequency of Br - Si at topological distance 7	2D Atom Pairs
	F07[Br-X]	Frequency of Br - X at topological distance 7	2D Atom Pairs
4544	F07[I-I]	Frequency of I - I at topological distance 7	2D Atom Pairs
4545	F07[I-B]	Frequency of I - B at topological distance 7	2D Atom Pairs
4546	F07[I-Si]	Frequency of I - Si at topological distance 7	2D Atom Pairs
	F07[I-X]	Frequency of I - X at topological distance 7	2D Atom Pairs
	F07[B-B]	Frequency of B - B at topological distance 7	2D Atom Pairs
			2D Atom Pairs
	F07[B-Si]	Frequency of B - Si at topological distance 7	
	F07[B-X]	Frequency of B - X at topological distance 7	2D Atom Pairs
	F07[Si-Si]	Frequency of Si - Si at topological distance 7	2D Atom Pairs
4552	F07[Si-X]	Frequency of Si - X at topological distance 7	2D Atom Pairs
4553	F07[X-X]	Frequency of X - X at topological distance 7	2D Atom Pairs
4554	F08[C-C]	Frequency of C - C at topological distance 8	2D Atom Pairs
	F08[C-N]	Frequency of C - N at topological distance 8	2D Atom Pairs
	F08[C-O]	Frequency of C - O at topological distance 8	2D Atom Pairs
	F08[C-S]	Frequency of C - S at topological distance 8	2D Atom Pairs
	F08[C-P]	Frequency of C - P at topological distance 8	2D Atom Pairs
	F08[C-F]	Frequency of C - F at topological distance 8	2D Atom Pairs
4560	F08[C-CI]	Frequency of C - CI at topological distance 8	2D Atom Pairs
4561	F08[C-Br]	Frequency of C - Br at topological distance 8	2D Atom Pairs
4562	F08[C-I]	Frequency of C - I at topological distance 8	2D Atom Pairs
	F08[C-B]	Frequency of C - B at topological distance 8	2D Atom Pairs
	F08[C-Si]	Frequency of C - Si at topological distance 8	2D Atom Pairs
	F08[C-X]	Frequency of C - X at topological distance 8	2D Atom Pairs
	F08[N-N]	Frequency of N - N at topological distance 8	2D Atom Pairs
	F08[N-O]	Frequency of N - O at topological distance 8	2D Atom Pairs
	F08[N-S]	Frequency of N - S at topological distance 8	2D Atom Pairs
	F08[N-P]	Frequency of N - P at topological distance 8	2D Atom Pairs
	F08[N-F]	Frequency of N - F at topological distance 8	2D Atom Pairs
4571	F08[N-CI]	Frequency of N - Cl at topological distance 8	2D Atom Pairs
	F08[N-Br]	Frequency of N - Br at topological distance 8	2D Atom Pairs
	F08[N-I]	Frequency of N - I at topological distance 8	2D Atom Pairs
	F08[N-B]	Frequency of N - B at topological distance 8	2D Atom Pairs
	F08[N-Si]	Frequency of N - Si at topological distance 8	2D Atom Pairs 2D Atom Pairs
	F08[N-X]	Frequency of N - X at topological distance 8	
	F08[O-O]	Frequency of O - O at topological distance 8	2D Atom Pairs
	F08[O-S]	Frequency of O - S at topological distance 8	2D Atom Pairs
	F08[O-P]	Frequency of O - P at topological distance 8	2D Atom Pairs
4580	F08[O-F]	Frequency of O - F at topological distance 8	2D Atom Pairs
	F08[O-CI]	Frequency of O - Cl at topological distance 8	2D Atom Pairs
	F08[O-Br]	Frequency of O - Br at topological distance 8	2D Atom Pairs
	F08[O-I]	Frequency of O - I at topological distance 8	2D Atom Pairs
	F08[O-B]	Frequency of O - Pat topological distance 8	2D Atom Pairs
			2D Atom Pairs
	F08[O-Si]	Frequency of O - Si at topological distance 8	
	F08[O-X]	Frequency of C - X at topological distance 8	2D Atom Pairs
	F08[S-S]	Frequency of S - S at topological distance 8	2D Atom Pairs
	F08[S-P]	Frequency of S - P at topological distance 8	2D Atom Pairs
	F08[S-F]	Frequency of S - F at topological distance 8	2D Atom Pairs
4590	F08[S-CI]	Frequency of S - Cl at topological distance 8	2D Atom Pairs
	F08[S-Br]	Frequency of S - Br at topological distance 8	2D Atom Pairs
	F08[S-I]	Frequency of S - I at topological distance 8	2D Atom Pairs
	F08[S-B]	Frequency of S - B at topological distance 8	2D Atom Pairs
			2D Atom Pairs
	F08[S-Si]	Frequency of S - Si at topological distance 8	
	F08[S-X]	Frequency of S - X at topological distance 8	2D Atom Pairs
	F08[P-P]	Frequency of P - P at topological distance 8	2D Atom Pairs
	F08[P-F]	Frequency of P - F at topological distance 8	2D Atom Pairs
4598	F08[P-CI]	Frequency of P - Cl at topological distance 8	2D Atom Pairs
4599	F08[P-Br]	Frequency of P - Br at topological distance 8	2D Atom Pairs
	F08[P-I]	Frequency of P - I at topological distance 8	2D Atom Pairs
	F08[P-B]	Frequency of P - B at topological distance 8	2D Atom Pairs
	F08[P-Si]	Frequency of P - Si at topological distance 8	2D Atom Pairs
	F08[P-X]	Frequency of P - X at topological distance 8	2D Atom Pairs
4004	F08[F-F]	Frequency of F - F at topological distance 8	2D Atom Pairs

4605	F08[F-CI]	Frequency of F - Cl at topological distance 8	2D Atom Pairs
4606	F08[F-Br]	Frequency of F - Br at topological distance 8	2D Atom Pairs
4607	F08[F-I]		2D Atom Pairs
4608	F08[F-B]		2D Atom Pairs
	F08[F-Si]		2D Atom Pairs
	F08[F-X]		2D Atom Pairs
	F08[CI-CI]		2D Atom Pairs
	F08[CI-Br]	- 1 3	2D Atom Pairs
	F08[CI-I]		2D Atom Pairs
	F08[CI-B]	· · ·	2D Atom Pairs
	F08[CI-Si]		2D Atom Pairs
	F08[CI-X]		2D Atom Pairs
	F08[Br-Br]		2D Atom Pairs
	F08[Br-I]		2D Atom Pairs
	F08[Br-B]	. ,	2D Atom Pairs
	F08[Br-Si]	- 1 3	2D Atom Pairs
	F08[Br-X]	· · ·	2D Atom Pairs
	F08[I-I]		2D Atom Pairs
	F08[I-B]		2D Atom Pairs
4624	F08[I-Si]	Frequency of I - Si at topological distance 8	2D Atom Pairs
4625	F08[I-X]	Frequency of I - X at topological distance 8	2D Atom Pairs
4626	F08[B-B]	Frequency of B - B at topological distance 8	2D Atom Pairs
4627	F08[B-Si]	Frequency of B - Si at topological distance 8	2D Atom Pairs
	F08[B-X]		2D Atom Pairs
	F08[Si-Si]		2D Atom Pairs
	F08[Si-X]		2D Atom Pairs
	F08[X-X]		2D Atom Pairs
			2D Atom Pairs
	F09[C-C] F09[C-N]		2D Atom Pairs
		- 1 3	
	F09[C-O]	· · ·	2D Atom Pairs
	F09[C-S]		2D Atom Pairs
	F09[C-P]		2D Atom Pairs
	F09[C-F]	· · ·	2D Atom Pairs
4638	F09[C-CI]	Frequency of C - Cl at topological distance 9	2D Atom Pairs
4639	F09[C-Br]		2D Atom Pairs
4640	F09[C-I]	Frequency of C - I at topological distance 9	2D Atom Pairs
4641	F09[C-B]	Frequency of C - B at topological distance 9	2D Atom Pairs
	F09[C-Si]		2D Atom Pairs
	F09[C-X]		2D Atom Pairs
	F09[N-N]	· · ·	2D Atom Pairs
	F09[N-O]		2D Atom Pairs
	F09[N-S]	. ,	2D Atom Pairs
	F09[N-P]		2D Atom Pairs
	F09[N-F]	· · ·	2D Atom Pairs
	F09[N-CI]	. ,	2D Atom Pairs
	F09[N-Br]		2D Atom Pairs
4651	F09[N-I]	Frequency of N - I at topological distance 9	2D Atom Pairs
4652	F09[N-B]	Frequency of N - B at topological distance 9	2D Atom Pairs
4653	F09[N-Si]	Frequency of N - Si at topological distance 9	2D Atom Pairs
4654	F09[N-X]	Frequency of N - X at topological distance 9	2D Atom Pairs
4655	F09[O-O]	Frequency of O - O at topological distance 9	2D Atom Pairs
	F09[O-S]		2D Atom Pairs
	F09[O-P]		2D Atom Pairs
	F09[O-F]		2D Atom Pairs
	F09[O-CI]		2D Atom Pairs
	F09[O-Br]	, ,	2D Atom Pairs
	F09[O-I]	. ,	2D Atom Pairs
	F09[O-B]		2D Atom Pairs
	F09[O-Si]	. ,	2D Atom Pairs 2D Atom Pairs
	F09[O-X]		
	F09[S-S]		2D Atom Pairs
	F09[S-P]		2D Atom Pairs
	F09[S-F]		2D Atom Pairs
	F09[S-CI]	- 1 7	2D Atom Pairs
	F09[S-Br]		2D Atom Pairs
	F09[S-I]		2D Atom Pairs
	F09[S-B]	-1, -1	2D Atom Pairs
	F09[S-Si]		2D Atom Pairs
	F09[S-X]		2D Atom Pairs
	F09[P-P]		2D Atom Pairs
4675	F09[P-F]	Frequency of P - F at topological distance 9	2D Atom Pairs
4676	F09[P-CI]	Frequency of P - Cl at topological distance 9	2D Atom Pairs
	F09[P-Br]		2D Atom Pairs
	F09[P-I]		2D Atom Pairs
	F09[P-B]	. ,	2D Atom Pairs
	F09[P-Si]		2D Atom Pairs
	F09[P-X]		2D Atom Pairs
	F09[F-F]		2D Atom Pairs
	F09[F-CI]		2D Atom Pairs
	F09[F-Br]		2D Atom Pairs
	F09[F-I]		2D Atom Pairs
	F09[F-B]		2D Atom Pairs
	F09[F-Si]		2D Atom Pairs
	F09[F-X]		2D Atom Pairs
	F09[CI-CI]		2D Atom Pairs
	F09[CI-Br]		2D Atom Pairs
	F09[CI-I]		2D Atom Pairs
	F09[CI-B]		2D Atom Pairs
	F09[CI-Si]		2D Atom Pairs
	F09[CI-X]	. ,	2D Atom Pairs
	F09[Br-Br]	. ,	2D Atom Pairs
	F09[Br-I]	. ,	2D Atom Pairs
4697	F09[Br-B]	Frequency of Br - B at topological distance 9	2D Atom Pairs
4698	F09[Br-Si]	Frequency of Br - Si at topological distance 9	2D Atom Pairs
	F09[Br-X]		2D Atom Pairs
	F09[I-I]		2D Atom Pairs

	F09[I-B]		2D Atom Pairs
4702	F09[I-Si]	Frequency of I - Si at topological distance 9	2D Atom Pairs
4703	F09[I-X]	Frequency of I - X at topological distance 9	2D Atom Pairs
4704	F09[B-B]	Frequency of B - B at topological distance 9	2D Atom Pairs
	F09[B-Si]	Frequency of B - Si at topological distance 9	2D Atom Pairs
	F09[B-X]		2D Atom Pairs
	F09[Si-Si]		2D Atom Pairs
	F09[Si-X]		2D Atom Pairs
	F09[X-X]	, ,	2D Atom Pairs
	F10[C-C]	. ,	2D Atom Pairs
4711	F10[C-N]	Frequency of C - N at topological distance 10	2D Atom Pairs
4712	F10[C-O]	Frequency of C - O at topological distance 10	2D Atom Pairs
4713	F10[C-S]	Frequency of C - S at topological distance 10	2D Atom Pairs
	F10[C-P]		2D Atom Pairs
	F10[C-F]	. ,	2D Atom Pairs
	F10[C-CI]	. ,	2D Atom Pairs
	F10[C-Br]	· · ·	2D Atom Pairs
	F10[C-I]		2D Atom Pairs
4719	F10[C-B]	Frequency of C - B at topological distance 10	2D Atom Pairs
4720	F10[C-Si]	Frequency of C - Si at topological distance 10	2D Atom Pairs
4721	F10[C-X]	Frequency of C - X at topological distance 10	2D Atom Pairs
	F10[N-N]		2D Atom Pairs
	F10[N-O]		2D Atom Pairs
	F10[N-S]		2D Atom Pairs
	F10[N-P]		2D Atom Pairs
	F10[N-F]		2D Atom Pairs
	F10[N-CI]	. ,	2D Atom Pairs
	F10[N-Br]	, ,	2D Atom Pairs
4729	F10[N-I]		2D Atom Pairs
4730	F10[N-B]	Frequency of N - B at topological distance 10	2D Atom Pairs
	F10[N-Si]		2D Atom Pairs
	F10[N-X]	. ,	2D Atom Pairs
	F10[O-O]		2D Atom Pairs
	F10[O-S]	. ,	2D Atom Pairs
		- 1 7	
	F10[O-P]	. ,	2D Atom Pairs
	F10[O-F]		2D Atom Pairs
4737	F10[O-CI]		2D Atom Pairs
4738	F10[O-Br]	Frequency of O - Br at topological distance 10	2D Atom Pairs
4739	F10[O-I]	Frequency of O - I at topological distance 10	2D Atom Pairs
4740	F10[O-B]	Frequency of O - B at topological distance 10	2D Atom Pairs
	F10[O-Si]		2D Atom Pairs
	F10[O-X]		2D Atom Pairs
	F10[S-S]		2D Atom Pairs
	F10[S-P]		2D Atom Pairs
	F10[S-F]		2D Atom Pairs
	F10[S-CI]	. ,	2D Atom Pairs
4747	F10[S-Br]	Frequency of S - Br at topological distance 10	2D Atom Pairs
4748	F10[S-I]	Frequency of S - I at topological distance 10	2D Atom Pairs
4749	F10[S-B]	Frequency of S - B at topological distance 10	2D Atom Pairs
4750	F10[S-Si]	Frequency of S - Si at topological distance 10	2D Atom Pairs
	F10[S-X]		2D Atom Pairs
	F10[P-P]		2D Atom Pairs
	F10[P-F]		2D Atom Pairs
	F10[P-CI]	- 1 - 3	2D Atom Pairs
	F10[P-Br]		2D Atom Pairs
	F10[P-I]	. ,	2D Atom Pairs
4757	F10[P-B]	Frequency of P - B at topological distance 10	2D Atom Pairs
4758	F10[P-Si]	Frequency of P - Si at topological distance 10	2D Atom Pairs
4759	F10[P-X]	Frequency of P - X at topological distance 10	2D Atom Pairs
4760	F10[F-F]	Frequency of F - F at topological distance 10	2D Atom Pairs
4761	F10[F-CI]	Frequency of F - Cl at topological distance 10	2D Atom Pairs
	F10[F-Br]		2D Atom Pairs
	F10[F-I]		2D Atom Pairs
	F10[F-B]	. ,	2D Atom Pairs
	F10[F-Si]	. ,	2D Atom Pairs
	F10[F-X]		2D Atom Pairs
	F10[CI-CI]	. ,	2D Atom Pairs
	F10[Cl-Br]		2D Atom Pairs
	F10[CI-I]		2D Atom Pairs
	F10[CI-B]		2D Atom Pairs
4771	F10[CI-Si]	Frequency of CI - Si at topological distance 10	2D Atom Pairs
	F10[CI-X]		2D Atom Pairs
	F10[Br-Br]		2D Atom Pairs
	F10[Br-I]	- 1 - 3	2D Atom Pairs
	F10[Br-B]		2D Atom Pairs
	F10[Br-Si]		2D Atom Pairs
	F10[Br-X]	. ,	2D Atom Pairs 2D Atom Pairs
		. ,	
	F10[I-I]	, , , , ,	2D Atom Pairs
	F10[I-B]	. ,	2D Atom Pairs
	F10[I-Si]		2D Atom Pairs
	F10[I-X]		2D Atom Pairs
4782	F10[B-B]	Frequency of B - B at topological distance 10	2D Atom Pairs
	F10[B-Si]	Frequency of B - Si at topological distance 10	2D Atom Pairs
	F10[B-X]		2D Atom Pairs
	F10[Si-Si]		2D Atom Pairs
	F10[Si-X]		2D Atom Pairs
	F10[X-X]		2D Atom Pairs
	G(NN)		3D Atom Pairs
			3D Atom Pairs
	G(N.O)		
	G(N.S)		3D Atom Pairs
	G(NP)		3D Atom Pairs
	G(NF)		3D Atom Pairs
	G(NCI)		3D Atom Pairs
4794	G(NBr)	sum of geometrical distances between NBr	3D Atom Pairs
	G(NI)		3D Atom Pairs
	G(OÓ)		3D Atom Pairs



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4700	G(OS)	sum of geometrical distances between OS	3D Atom Pairs
	G(OP)	sum of geometrical distances between OP	3D Atom Pairs
	G(OF)	sum of geometrical distances between OF	3D Atom Pairs
	G(OCI)	sum of geometrical distances between OCl	3D Atom Pairs
	G(OBr)	sum of geometrical distances between OBr	3D Atom Pairs
	G(OI)	sum of geometrical distances between OI	3D Atom Pairs
	G(SS) G(SP)	sum of geometrical distances between SS	3D Atom Pairs 3D Atom Pairs
		sum of geometrical distances between SP	
	G(SF)	sum of geometrical distances between SF	3D Atom Pairs
	G(SCI)	sum of geometrical distances between SCl	3D Atom Pairs
	G(SBr)	sum of geometrical distances between SBr	3D Atom Pairs
	G(SI)	sum of geometrical distances between SI	3D Atom Pairs
	G(PP) G(PF)	sum of geometrical distances between PP	3D Atom Pairs
	' '	sum of geometrical distances between PF	3D Atom Pairs
	G(PCI)	sum of geometrical distances between PCl	3D Atom Pairs
	G(PBr)	sum of geometrical distances between PBr	3D Atom Pairs 3D Atom Pairs
	G(PI) G(FF)	sum of geometrical distances between PI	3D Atom Pairs
		sum of geometrical distances between FF sum of geometrical distances between FCl	3D Atom Pairs
	G(FCl) G(FBr)		3D Atom Pairs
	G(FI)	sum of geometrical distances between FBr sum of geometrical distances between FI	3D Atom Pairs
			3D Atom Pairs
	G(CL.CI)	sum of geometrical distances between ClCl	3D Atom Pairs
	G(CL.)	sum of geometrical distances between Cl. Br	3D Atom Pairs
	G(Cll) G(BrBr)	sum of geometrical distances between Cll sum of geometrical distances between BrBr	3D Atom Pairs
	G(BrI)	sum of geometrical distances between Brl	3D Atom Pairs
	G(II)	sum of geometrical distances between II	3D Atom Pairs
	qpmax		Charge descriptors
	qnmax	maximum positive charge	Charge descriptors
4826		maximum negative charge total positive charge	Charge descriptors
	Qneg		
4828		total negative charge total absolute charge (electronic charge index - ECI)	Charge descriptors Charge descriptors
	Qmean		Charge descriptors
4830		mean absolute charge (charge polarization) total squared charge	Charge descriptors
	RPCG	relative positive charge	Charge descriptors
	RNCG	relative negative charge	Charge descriptors
4833		submolecular polarity parameter	Charge descriptors
4834		topographic electronic descriptor	Charge descriptors
4835		topographic electronic descriptor (bond resctricted)	Charge descriptors
	PCWTE1	partial charge weighted topological electronic index	Charge descriptors
	PCWTE2	partial charge weighted topological electronic index (bond resctricted)	Charge descriptors
4838		local dipole index	Charge descriptors
4839		unsaturation count	Molecular properties
4840		unsaturation index	Molecular properties
4841		hydrophilic factor	Molecular properties
4842		Ghose-Crippen molar refractivity	Molecular properties
			Molecular properties
	I DSA/N(I)	tonological notar surface area using N.O. notar contributions	Molecular properties
	TPSA(NO)	topological polar surface area using N,O polar contributions	Molecular properties
4844	TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions	Molecular properties
4844 4845	TPSA(Tot) MLOGP	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP)	Molecular properties Molecular properties
4844 4845 4846	TPSA(Tot) MLOGP MLOGP2	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2)	Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847	TPSA(Tot) MLOGP MLOGP2 ALOGP	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP)	Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP ²) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP)	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849 4850	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849 4850 4851	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849 4850 4851 4852	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849 4850 4851 4852 4853	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon Vx VvdwMG	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume	Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties Molecular properties
4844 4845 4846 4847 4848 4849 4850 4851 4852 4853 4854	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwMG PDI	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I)	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856 4857	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTD48	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I)	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856 4857 4858	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTF96 BLTA96	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I)	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856 4857	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTD48	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I)	Molecular properties
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856 4857 4858 4859 4860	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTT96 BLTD48 BLTD48 BLTA96 cR05	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP^3) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4852 4853 4856 4857 4858 4859 4860 4860	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTT96 BLTD48 BLTA96 cRo5 DLS_01	topological polar surface area using N.O.S.P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules)	Molecular properties Drug-like indices Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4852 4853 4856 4857 4858 4859 4860 4861	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAtot SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTF96 BLTD48 BLTA96 cRo5 DLS_01 DLS_02	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Oprea et al. (6 rules)	Molecular properties Drug-like indices Drug-like indices Drug-like indices
4844 4845 4846 4847 4850 4851 4852 4853 4854 4855 4856 4857 4858 4859 4860 4861 4862 4863	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTD48 BLTA96 cR05 DLS_01 DLS_02 DLS_03	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Oprea et al. (6 rules)	Molecular properties Drug-like indices Drug-like indices Drug-like indices Drug-like indices
4844 4845 4846 4847 4850 4851 4852 4853 4854 4855 4856 4857 4858 4860 4861 4862 4863	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTD48 BLTD48 BLTA96 cR05 DLS_01 DLS_02 DLS_03 DLS_04	topological polar surface area using N.O.S.P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Walters et al. (6 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4856 4857 4858 4859 4860 4861 4862 4863 4864 4865	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTF96 BLTP96 BLTD48 BLTA96 cRo5 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Walters et al. (7 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Chen et al. (7 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4855 4856 4859 4860 4861 4862 4863 4864 4865 4865	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 SAtot SAacc SAdon Vx VvdwMG VvdwZAZ PDI BLTF96 BLTF96 BLTD48 BLTA96 cR05 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05 DLS_06	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from McGowan-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Rishton (6 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4850 4851 4852 4853 4854 4855 4856 4857 4858 4860 4861 4862 4863 4864 4864 4866	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTF96 BLTD48 BLTA96 cR05 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05 DLS_06 DLS_07	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP^2) Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from McGowan volume Van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Upinski (4 rules) modified drug-like score from Waters et al. (6 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Zheng et al. (2 rules) modified drug-like score from Zheng et al. (2 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Rishton (6 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4855 4856 4856 4856 4861 4862 4863 4864 4865 4866 4867 4868	TPSA(Tot) MLOGP MLOGP2 ALOGP ALOGP2 ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTP96 BLTD48 BLTA96 cRo5 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05 DLS_06 DLS_07 DLS_cons	topological polar surface area using N.O.S.P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Zheng et al. (2 rules) modified drug-like score from Rishton (6 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4852 4853 4854 4856 4857 4860 4861 4862 4863 4864 4865 4866 4867 4868	TPSA(Tot) MLOGP MLOGP2 ALOGP2 ALOGP2 ALOGP2 SAtot SAtot SAdon VX VvdwMG VvdwZAZ PDI BLTF96 BLTF96 BLTD48 BLTA96 cRo5 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05 DLS_06 DLS_07 DLS_07 DLS_07 DLS_07 DLS_07 DLS_07 DLS_07 DLS_07 DLS_07	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Walters et al. (7 rules) modified drug-like score from Enen et al. (7 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Neber et al. (2 rules) DRAGON consensus drug-like score modified lead-like score from Congreve et al. (6 rules)	Molecular properties Drug-like indices
4844 4845 4846 4847 4848 4850 4851 4855 4855 4856 4857 4858 4859 4860 4861 4862 4863 4864 4865 4866 4867 4868 4869 4871	TPSA(Tot) MLOGP MLOGP MLOGP2 ALOGP ALOGP2 ALOGP2 SAtot SAacc SAdon VX VvdwMG VvdwZAZ PDI BLTF96 BLTP96 BLTD48 BLTA96 cRo5 DLS_01 DLS_02 DLS_03 DLS_04 DLS_05 DLS_06 DLS_07 DLS_07 DLS_07 DLS_07 DLS_001 LLS_01 LLS_02 CMC-80 CMC-80 CMC-50	topological polar surface area using N,O,S,P polar contributions Moriguchi octanol-water partition coeff. (logP) squared Moriguchi octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP) squared Ghose-Crippen octanol-water partition coeff. (logP^2) total surface area from P_VSA-like descriptors surface area of acceptor atoms from P_VSA-like descriptors surface area of donor atoms from P_VSA-like descriptors McGowan volume van der Waals volume from McGowan volume van der Waals volume from McGowan volume van der Waals volume from Zhao-Abraham-Zissimos equation packing density index Verhaar Fish base-line toxicity from MLOGP (mmol/I) Verhaar Daphnia base-line toxicity from MLOGP (mmol/I) Verhaar Algae base-line toxicity from MLOGP (mmol/I) Complementary Lipinski Alert index modified drug-like score from Lipinski (4 rules) modified drug-like score from Walters et al. (6 rules) modified drug-like score from Chen et al. (7 rules) modified drug-like score from Zheng et al. (2 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Rishton (6 rules) modified drug-like score from Veber et al. (2 rules) DRAGON consensus drug-like score modified lead-like score from Congreve et al. (6 rules) modified lead-like score from Monge et al. (6 rules)	Molecular properties Drug-like indices
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