**Supplementary 1:** Chemicals used in the development of prediction models **(**Page no. 1-91)

|  |  |  |
| --- | --- | --- |
| **S. No.** | **Mol ID** | **Class** |
| 1 | 1728-95-6 | Mutagen |
| 2 | 91-08-7 | Mutagen |
| 3 | 89786-04-9 | Nonmutagen |
| 4 | 2439-35-2 | Nonmutagen |
| 5 | 95-94-3 | Nonmutagen |
| 6 | 120314-14-9 | Mutagen |
| 7 | 146795-42-8 | Mutagen |
| 8 | 119-41-5 | Nonmutagen |
| 9 | 614-00-6 | Mutagen |
| 10 | 77996-03-3 | Mutagen |
| 11 | 123-01-3 | Nonmutagen |
| 12 | 53478-38-9 | Mutagen |
| 13 | 1836-75-5 | Mutagen |
| 14 | 329-71-5 | Mutagen |
| 15 | 108-64-5 | Nonmutagen |
| 16 | 146177-59-5 | Mutagen |
| 17 | 106264-79-3 | Mutagen |
| 18 | 88488-97-5 | Mutagen |
| 19 | 61203-01-8 | Mutagen |
| 20 | 112-24-3 | Mutagen |
| 21 | 2849-98-1 | Nonmutagen |
| 22 | 16423-19-1 | Nonmutagen |
| 23 | 97-90-5 | Nonmutagen |
| 24 | 50438-75-0 | Mutagen |
| 25 | 126983-60-6 | Mutagen |
| 26 | 89-98-5 | Nonmutagen |
| 27 | 82-62-2 | Nonmutagen |
| 28 | 97606-15-0 | Mutagen |
| 29 | 91-53-2 | Nonmutagen |
| 30 | 117-81-7 | Nonmutagen |
| 31 | 1928-43-4 | Nonmutagen |
| 32 | 507-55-1 | Nonmutagen |
| 33 | 5042-54-6 | Mutagen |
| 34 | 396-01-0 | Nonmutagen |
| 35 | 120-61-6 | Nonmutagen |
| 36 | 3807-77-0 | Mutagen |
| 37 | 612-59-9 | Nonmutagen |
| 38 | 13675-34-8 | Nonmutagen |
| 39 | 71628-96-1 | Mutagen |
| 40 | 4629-58-7 | Mutagen |
| 41 | 142438-73-1 | Mutagen |
| 42 | 500-38-9 | Nonmutagen |
| 43 | 97-24-5 | Nonmutagen |
| 44 | 5634-39-9 | Mutagen |
| 45 | 93-68-5 | Nonmutagen |
| 46 | 109-99-9 | Nonmutagen |
| 47 | 88133-11-3 | Nonmutagen |
| 48 | 103942-97-8 | Mutagen |
| 49 | 60-23-1 | Nonmutagen |
| 50 | 119169-78-7 | Nonmutagen |
| 51 | 92-88-6 | Nonmutagen |
| 52 | 106-38-7 | Nonmutagen |
| 53 | 4985-70-0 | Nonmutagen |
| 54 | 482-27-9 | Nonmutagen |
| 55 | 86-73-7 | Nonmutagen |
| 56 | 17924-92-4 | Nonmutagen |
| 57 | 95-64-7 | Mutagen |
| 58 | 67587-52-4 | Mutagen |
| 59 | 610-14-0 | Mutagen |
| 60 | 17341-40-1 | Nonmutagen |
| 61 | 105-58-8 | Nonmutagen |
| 62 | 100757-60-6 | Nonmutagen |
| 63 | 16069-36-6 | Nonmutagen |
| 64 | 140-08-9 | Mutagen |
| 65 | 6066-82-6 | Nonmutagen |
| 66 | 10605-21-7 | Mutagen |
| 67 | 68743-68-0 | Mutagen |
| 68 | 505-29-3 | Mutagen |
| 69 | 135-68-2 | Mutagen |
| 70 | 484-23-1 | Mutagen |
| 71 | 114460-39-8 | Mutagen |
| 72 | 104-78-9 | Nonmutagen |
| 73 | 39720-27-9 | Mutagen |
| 74 | 6149-33-3 | Mutagen |
| 75 | 123-92-2 | Nonmutagen |
| 76 | 36712-34-2 | Mutagen |
| 77 | 54827-17-7 | Nonmutagen |
| 78 | 91-23-6 | Mutagen |
| 79 | 218-19-9 | Mutagen |
| 80 | 111-14-8 | Nonmutagen |
| 81 | 115664-50-1 | Mutagen |
| 82 | 6449-35-0 | Mutagen |
| 83 | 88-88-0 | Mutagen |
| 84 | 68140-48-7 | Nonmutagen |
| 85 | 77-92-9 | Nonmutagen |
| 86 | 51640-90-5 | Mutagen |
| 87 | 75-11-6 | Nonmutagen |
| 88 | 568-75-2 | Mutagen |
| 89 | 2541-69-7 | Mutagen |
| 90 | 4450-68-4 | Mutagen |
| 91 | 5000-65-7 | Nonmutagen |
| 92 | 77121-90-5 | Mutagen |
| 93 | 138580-48-0 | Mutagen |
| 94 | 03-09-6268 | Mutagen |
| 95 | 96563-10-9 | Mutagen |
| 96 | 2508-20-5 | Mutagen |
| 97 | 100-37-8 | Nonmutagen |
| 98 | 4825-86-9 | Nonmutagen |
| 99 | 1436-34-6 | Nonmutagen |
| 100 | 105579-74-6 | Mutagen |
| 101 | 96-99-1 | Mutagen |
| 102 | 74-31-7 | Mutagen |
| 103 | 142044-37-9 | Mutagen |
| 104 | 462-95-3 | Nonmutagen |
| 105 | 615-05-4 | Mutagen |
| 106 | 868-77-9 | Nonmutagen |
| 107 | 491-80-5 | Nonmutagen |
| 108 | 82389-38-6 | Mutagen |
| 109 | 99-75-2 | Nonmutagen |
| 110 | 108-70-3 | Nonmutagen |
| 111 | 146177-65-3 | Mutagen |
| 112 | 57-13-6 | Nonmutagen |
| 113 | 29916-56-1 | Mutagen |
| 114 | 109-69-3 | Nonmutagen |
| 115 | 109143-20-6 | Mutagen |
| 116 | 98-95-3 | Nonmutagen |
| 117 | 125239-64-7 | Mutagen |
| 118 | 156215-58-6 | Mutagen |
| 119 | 83-67-0 | Nonmutagen |
| 120 | 108-89-4 | Nonmutagen |
| 121 | 93780-96-2 | Mutagen |
| 122 | 830-96-6 | Nonmutagen |
| 123 | 578-06-3 | Mutagen |
| 124 | 42200-33-9 | Nonmutagen |
| 125 | 484-78-6 | Nonmutagen |
| 126 | 590-88-5 | Nonmutagen |
| 127 | 117929-13-2 | Mutagen |
| 128 | 02-02-1953 | Nonmutagen |
| 129 | 3442-62-4 | Mutagen |
| 130 | 2012-00-2 | Mutagen |
| 131 | 102822-04-8 | Mutagen |
| 132 | 10147-37-2 | Mutagen |
| 133 | 111-69-3 | Nonmutagen |
| 134 | 62450-07-1 | Mutagen |
| 135 | 33037-07-9 | Mutagen |
| 136 | 161697-03-6 | Mutagen |
| 137 | 15299-08-8 | Mutagen |
| 138 | 5466-77-3 | Nonmutagen |
| 139 | 4098-71-9 | Nonmutagen |
| 140 | 99-09-2 | Mutagen |
| 141 | 5470-37-1 | Nonmutagen |
| 142 | 41533-75-9 | Mutagen |
| 143 | 110419-21-1 | Mutagen |
| 144 | 133831-60-4 | Mutagen |
| 145 | 13593-03-8 | Nonmutagen |
| 146 | 78-42-2 | Nonmutagen |
| 147 | 6884-87-3 | Nonmutagen |
| 148 | 116374-65-3 | Mutagen |
| 149 | 113698-18-3 | Mutagen |
| 150 | 123-73-9 | Mutagen |
| 151 | 3930-19-6 | Mutagen |
| 152 | 4430-25-5 | Nonmutagen |
| 153 | 609-19-8 | Nonmutagen |
| 154 | 69177-41-9 | Mutagen |
| 155 | 4792-83-0 | Nonmutagen |
| 156 | 116505-02-3 | Mutagen |
| 157 | 96910-73-5 | Mutagen |
| 158 | 92-94-4 | Nonmutagen |
| 159 | 50-32-8 | Mutagen |
| 160 | 90-13-1 | Mutagen |
| 161 | 212-54-4 | Mutagen |
| 162 | 26530-20-1 | Nonmutagen |
| 163 | 321-14-2 | Nonmutagen |
| 164 | 95-70-5 | Mutagen |
| 165 | 3397-62-4 | Nonmutagen |
| 166 | 6358-53-8 | Mutagen |
| 167 | 607-59-0 | Mutagen |
| 168 | 96-69-5 | Nonmutagen |
| 169 | 512-56-1 | Mutagen |
| 170 | 525-03-1 | Nonmutagen |
| 171 | 598-55-0 | Nonmutagen |
| 172 | 17902-23-7 | Nonmutagen |
| 173 | 3018-12-0 | Mutagen |
| 174 | 32692-19-6 | Mutagen |
| 175 | 146795-37-1 | Mutagen |
| 176 | 8003-03-0 | Nonmutagen |
| 177 | 104445-28-5 | Mutagen |
| 178 | 637-69-4 | Nonmutagen |
| 179 | 106063-42-7 | Mutagen |
| 180 | 93-08-3 | Nonmutagen |
| 181 | 119-36-8 | Mutagen |
| 182 | 15131-84-7 | Mutagen |
| 183 | 610-39-9 | Mutagen |
| 184 | 112575-91-4 | Mutagen |
| 185 | 111712-47-1 | Mutagen |
| 186 | 106449-56-3 | Nonmutagen |
| 187 | 1672-88-4 | Mutagen |
| 188 | 105650-23-5 | Mutagen |
| 189 | 479-13-0 | Nonmutagen |
| 190 | 14925-39-4 | Mutagen |
| 191 | 27113-22-0 | Nonmutagen |
| 192 | 118-56-9 | Nonmutagen |
| 193 | 111-20-6 | Nonmutagen |
| 194 | 89784-39-4 | Mutagen |
| 195 | 22608-53-3 | Nonmutagen |
| 196 | 617-48-1 | Nonmutagen |
| 197 | 13707-88-5 | Nonmutagen |
| 198 | 602-38-0 | Mutagen |
| 199 | 33089-36-0 | Nonmutagen |
| 200 | 100-43-6 | Nonmutagen |
| 201 | 61740-00-9 | Mutagen |
| 202 | 1928-38-7 | Nonmutagen |
| 203 | 85-33-6 | Mutagen |
| 204 | 75-36-5 | Nonmutagen |
| 205 | 621-52-3 | Nonmutagen |
| 206 | 693-98-1 | Nonmutagen |
| 207 | 67730-11-4 | Mutagen |
| 208 | 565-20-8 | Nonmutagen |
| 209 | 15088-70-7 | Nonmutagen |
| 210 | 24496-65-9 | Mutagen |
| 211 | 346-18-9 | Nonmutagen |
| 212 | 1761-71-3 | Nonmutagen |
| 213 | 110-59-8 | Nonmutagen |
| 214 | 68162-37-8 | Mutagen |
| 215 | 6257-64-3 | Nonmutagen |
| 216 | 103393-72-2 | Mutagen |
| 217 | 97-00-7 | Mutagen |
| 218 | 57309-27-0 | Nonmutagen |
| 219 | 836-37-3 | Mutagen |
| 220 | 123-32-0 | Nonmutagen |
| 221 | 64188-64-3 | Mutagen |
| 222 | 29590-42-9 | Nonmutagen |
| 223 | 118-92-3 | Nonmutagen |
| 224 | 61788-44-1 | Nonmutagen |
| 225 | 114454-59-0 | Mutagen |
| 226 | 51325-91-8 | Mutagen |
| 227 | 06-08-2426 | Mutagen |
| 228 | 603-54-3 | Nonmutagen |
| 229 | 555-68-0 | Mutagen |
| 230 | 112-55-0 | Nonmutagen |
| 231 | 693-13-0 | Nonmutagen |
| 232 | 127-07-1 | Mutagen |
| 233 | 503-09-3 | Mutagen |
| 234 | 27946-19-6 | Mutagen |
| 235 | 2226-96-2 | Mutagen |
| 236 | 54818-87-0 | Mutagen |
| 237 | 6358-23-2 | Mutagen |
| 238 | 80115-73-7 | Mutagen |
| 239 | 501-30-4 | Mutagen |
| 240 | 2224-15-9 | Mutagen |
| 241 | 91-84-9 | Nonmutagen |
| 242 | 126-27-2 | Nonmutagen |
| 243 | 151-56-4 | Mutagen |
| 244 | 1522-92-5 | Mutagen |
| 245 | 2921-88-2 | Nonmutagen |
| 246 | 108-10-1 | Nonmutagen |
| 247 | 52898-98-3 | Mutagen |
| 248 | 139953-77-8 | Mutagen |
| 249 | 21229-99-2 | Mutagen |
| 250 | 104-54-1 | Nonmutagen |
| 251 | 626-43-7 | Nonmutagen |
| 252 | 73341-53-4 | Mutagen |
| 253 | 129-03-3 | Nonmutagen |
| 254 | 119-06-2 | Nonmutagen |
| 255 | 109-09-1 | Mutagen |
| 256 | 396-32-7 | Mutagen |
| 257 | 150-76-5 | Nonmutagen |
| 258 | 58-54-8 | Nonmutagen |
| 259 | 112022-06-7 | Mutagen |
| 260 | 78-67-1 | Nonmutagen |
| 261 | 2562-38-1 | Mutagen |
| 262 | 106-50-3 | Mutagen |
| 263 | 159092-71-4 | Mutagen |
| 264 | 33611-88-0 | Mutagen |
| 265 | 100-13-0 | Mutagen |
| 266 | 1116-40-1 | Nonmutagen |
| 267 | 87-84-3 | Nonmutagen |
| 268 | 132335-20-7 | Mutagen |
| 269 | 3688-53-7 | Mutagen |
| 270 | 548-83-4 | Nonmutagen |
| 271 | 148193-30-0 | Mutagen |
| 272 | 96839-34-8 | Nonmutagen |
| 273 | 60-33-3 | Nonmutagen |
| 274 | 129176-05-2 | Mutagen |
| 275 | 116-66-5 | Nonmutagen |
| 276 | 502-65-8 | Nonmutagen |
| 277 | 578-67-6 | Mutagen |
| 278 | 20153-98-4 | Nonmutagen |
| 279 | 28124-29-0 | Mutagen |
| 280 | 83905-01-5 | Nonmutagen |
| 281 | 146795-43-9 | Mutagen |
| 282 | 2855-19-8 | Nonmutagen |
| 283 | 115-86-6 | Nonmutagen |
| 284 | 58-90-2 | Nonmutagen |
| 285 | 68299-98-9 | Nonmutagen |
| 286 | 581-47-5 | Mutagen |
| 287 | 89-80-5 | Mutagen |
| 288 | 1635-63-8 | Nonmutagen |
| 289 | 62-50-0 | Mutagen |
| 290 | 59-89-2 | Mutagen |
| 291 | 159394-73-7 | Mutagen |
| 292 | 1982-67-8 | Nonmutagen |
| 293 | 18829-55-5 | Mutagen |
| 294 | 820-75-7 | Mutagen |
| 295 | 41044-12-6 | Nonmutagen |
| 296 | 19600-63-6 | Mutagen |
| 297 | 102-28-3 | Mutagen |
| 298 | 08-09-4350 | Nonmutagen |
| 299 | 13345-23-8 | Mutagen |
| 300 | 133-18-6 | Nonmutagen |
| 301 | 2531-84-2 | Mutagen |
| 302 | 28166-06-5 | Mutagen |
| 303 | 126983-61-7 | Mutagen |
| 304 | 91423-46-0 | Mutagen |
| 305 | 81424-67-1 | Mutagen |
| 306 | 709-49-9 | Mutagen |
| 307 | 316-14-3 | Mutagen |
| 308 | 96-09-3 | Mutagen |
| 309 | 74367-78-5 | Mutagen |
| 310 | 1013-96-3 | Nonmutagen |
| 311 | 16430-32-3 | Mutagen |
| 312 | 2851-80-1 | Nonmutagen |
| 313 | 542-75-6 | Mutagen |
| 314 | 1516-21-8 | Mutagen |
| 315 | 628-94-4 | Nonmutagen |
| 316 | 65-45-2 | Nonmutagen |
| 317 | 115453-71-9 | Nonmutagen |
| 318 | 142129-81-5 | Nonmutagen |
| 319 | 166664-83-1 | Nonmutagen |
| 320 | 18234-46-3 | Mutagen |
| 321 | 4812-40-2 | Mutagen |
| 322 | 14698-29-4 | Mutagen |
| 323 | 529-20-4 | Nonmutagen |
| 324 | 519-23-3 | Mutagen |
| 325 | 102234-07-1 | Mutagen |
| 326 | 525-64-4 | Mutagen |
| 327 | 644-21-3 | Mutagen |
| 328 | 102059-18-7 | Mutagen |
| 329 | 621-77-2 | Nonmutagen |
| 330 | 89930-59-6 | Mutagen |
| 331 | 116169-87-0 | Mutagen |
| 332 | 2942-42-9 | Mutagen |
| 333 | 2598-29-0 | Nonmutagen |
| 334 | 92-70-6 | Nonmutagen |
| 335 | 94500-54-6 | Mutagen |
| 336 | 52411-33-3 | Mutagen |
| 337 | 106-20-7 | Nonmutagen |
| 338 | 6190-65-4 | Nonmutagen |
| 339 | 288-32-4 | Nonmutagen |
| 340 | 202-33-5 | Mutagen |
| 341 | 35144-55-9 | Nonmutagen |
| 342 | 144561-63-7 | Mutagen |
| 343 | 607-35-2 | Mutagen |
| 344 | 60-24-2 | Nonmutagen |
| 345 | 126-33-0 | Nonmutagen |
| 346 | 96-45-7 | Mutagen |
| 347 | 51630-58-1 | Nonmutagen |
| 348 | 13952-84-6 | Nonmutagen |
| 349 | 17804-35-2 | Nonmutagen |
| 350 | 16683-64-0 | Mutagen |
| 351 | 101-84-8 | Nonmutagen |
| 352 | 789-47-9 | Mutagen |
| 353 | 134998-76-8 | Mutagen |
| 354 | 2303-16-4 | Mutagen |
| 355 | 27729-95-9 | Mutagen |
| 356 | 141-91-3 | Mutagen |
| 357 | 02-09-7364 | Mutagen |
| 358 | 22316-47-8 | Nonmutagen |
| 359 | 105-59-9 | Nonmutagen |
| 360 | 2835-97-4 | Nonmutagen |
| 361 | 101688-02-2 | Mutagen |
| 362 | 609-31-4 | Nonmutagen |
| 363 | 2106-54-9 | Nonmutagen |
| 364 | 103-80-0 | Mutagen |
| 365 | 951-80-4 | Mutagen |
| 366 | 224-42-0 | Mutagen |
| 367 | 63019-38-5 | Mutagen |
| 368 | 218-01-9 | Mutagen |
| 369 | 14064-55-2 | Mutagen |
| 370 | 39413-05-3 | Nonmutagen |
| 371 | 6149-34-4 | Mutagen |
| 372 | 965-52-6 | Mutagen |
| 373 | 82-33-7 | Mutagen |
| 374 | 36712-35-3 | Mutagen |
| 375 | 24424-99-5 | Nonmutagen |
| 376 | 87-90-1 | Nonmutagen |
| 377 | 101-18-8 | Nonmutagen |
| 378 | 5806-00-8 | Nonmutagen |
| 379 | 115664-51-2 | Mutagen |
| 380 | 3118-97-6 | Mutagen |
| 381 | 88-89-1 | Mutagen |
| 382 | 206-44-0 | Mutagen |
| 383 | 75-12-7 | Nonmutagen |
| 384 | 96563-11-0 | Mutagen |
| 385 | 64920-31-6 | Mutagen |
| 386 | 55-18-5 | Mutagen |
| 387 | 90-44-8 | Mutagen |
| 388 | 120-32-1 | Nonmutagen |
| 389 | 42397-64-8 | Mutagen |
| 390 | 758-17-8 | Nonmutagen |
| 391 | 97576-08-4 | Mutagen |
| 392 | 54954-12-0 | Mutagen |
| 393 | 136-85-6 | Nonmutagen |
| 394 | 22089-22-1 | Mutagen |
| 395 | 3531-19-9 | Mutagen |
| 396 | 96383-86-7 | Mutagen |
| 397 | 124-07-2 | Nonmutagen |
| 398 | 27451-21-4 | Nonmutagen |
| 399 | 5307-00-6 | Nonmutagen |
| 400 | 99-76-3 | Nonmutagen |
| 401 | 60129-67-1 | Mutagen |
| 402 | 7269-57-0 | Mutagen |
| 403 | 57-14-7 | Mutagen |
| 404 | 885-11-0 | Mutagen |
| 405 | 154-93-8 | Mutagen |
| 406 | 499-12-7 | Nonmutagen |
| 407 | 202-03-9 | Mutagen |
| 408 | 24463-15-8 | Mutagen |
| 409 | 63018-94-0 | Mutagen |
| 410 | 98-96-4 | Nonmutagen |
| 411 | 125239-65-8 | Mutagen |
| 412 | 3132-64-7 | Mutagen |
| 413 | 62-75-9 | Mutagen |
| 414 | 92-59-1 | Nonmutagen |
| 415 | 528-29-0 | Mutagen |
| 416 | 52101-49-2 | Mutagen |
| 417 | 642-31-9 | Nonmutagen |
| 418 | 26651-23-0 | Mutagen |
| 419 | 1464-53-5 | Mutagen |
| 420 | 584-48-5 | Mutagen |
| 421 | 26196-45-2 | Mutagen |
| 422 | 117929-14-3 | Mutagen |
| 423 | 100593-23-5 | Mutagen |
| 424 | 33203-82-6 | Mutagen |
| 425 | 646-06-0 | Nonmutagen |
| 426 | 100-74-3 | Mutagen |
| 427 | 10443-65-9 | Nonmutagen |
| 428 | 627-18-9 | Mutagen |
| 429 | 230-27-3 | Mutagen |
| 430 | 1321-74-0 | Nonmutagen |
| 431 | 4569-77-1 | Mutagen |
| 432 | 161697-04-7 | Mutagen |
| 433 | 98-11-3 | Nonmutagen |
| 434 | 107097-80-3 | Nonmutagen |
| 435 | 1070-70-8 | Nonmutagen |
| 436 | 496-72-0 | Mutagen |
| 437 | 103-50-4 | Nonmutagen |
| 438 | 632-79-1 | Nonmutagen |
| 439 | 102000-59-9 | Mutagen |
| 440 | 25057-89-0 | Nonmutagen |
| 441 | 6281-23-8 | Mutagen |
| 442 | 133831-61-5 | Mutagen |
| 443 | 53-94-1 | Mutagen |
| 444 | 134785-76-5 | Mutagen |
| 445 | 2310-17-0 | Nonmutagen |
| 446 | 313-80-4 | Mutagen |
| 447 | 619-17-0 | Mutagen |
| 448 | 116374-66-4 | Mutagen |
| 449 | 102-70-5 | Nonmutagen |
| 450 | 71711-58-5 | Mutagen |
| 451 | 103-69-5 | Nonmutagen |
| 452 | 5869-25-0 | Mutagen |
| 453 | 120693-41-6 | Mutagen |
| 454 | 84736-60-7 | Mutagen |
| 455 | 603-85-0 | Nonmutagen |
| 456 | 7417-67-6 | Mutagen |
| 457 | 3032-55-1 | Nonmutagen |
| 458 | 42017-89-0 | Nonmutagen |
| 459 | 55804-66-5 | Nonmutagen |
| 460 | 109460-96-0 | Nonmutagen |
| 461 | 5443-49-2 | Mutagen |
| 462 | 101-90-6 | Mutagen |
| 463 | 50-33-9 | Nonmutagen |
| 464 | 584-84-9 | Mutagen |
| 465 | 110-05-4 | Nonmutagen |
| 466 | 132335-15-0 | Mutagen |
| 467 | 527-85-5 | Nonmutagen |
| 468 | 80-43-3 | Nonmutagen |
| 469 | 109-21-7 | Nonmutagen |
| 470 | 305-03-3 | Mutagen |
| 471 | 142-96-1 | Nonmutagen |
| 472 | 4067-16-7 | Mutagen |
| 473 | 600-24-8 | Nonmutagen |
| 474 | 24305-27-9 | Nonmutagen |
| 475 | 21738-42-1 | Mutagen |
| 476 | 146795-38-2 | Mutagen |
| 477 | 17683-09-9 | Mutagen |
| 478 | 63-25-2 | Mutagen |
| 479 | 645-62-5 | Nonmutagen |
| 480 | 104-85-8 | Nonmutagen |
| 481 | 687-48-9 | Mutagen |
| 482 | 89-75-8 | Mutagen |
| 483 | 253-52-1 | Nonmutagen |
| 484 | 125676-80-4 | Mutagen |
| 485 | 83-38-5 | Nonmutagen |
| 486 | 498-02-2 | Nonmutagen |
| 487 | 28995-89-3 | Mutagen |
| 488 | 333-27-7 | Mutagen |
| 489 | 70853-94-0 | Mutagen |
| 490 | 88-95-9 | Mutagen |
| 491 | 78-98-8 | Mutagen |
| 492 | 97-86-9 | Nonmutagen |
| 493 | 71432-00-3 | Mutagen |
| 494 | 1948-33-0 | Nonmutagen |
| 495 | 100-44-7 | Mutagen |
| 496 | 92180-79-5 | Mutagen |
| 497 | 3385-21-5 | Nonmutagen |
| 498 | 51483-40-0 | Mutagen |
| 499 | 94-25-7 | Nonmutagen |
| 500 | 99217-04-6 | Mutagen |
| 501 | 96287-03-5 | Mutagen |
| 502 | 482-89-3 | Mutagen |
| 503 | 3319-31-1 | Nonmutagen |
| 504 | 99-82-1 | Nonmutagen |
| 505 | 2564-65-0 | Mutagen |
| 506 | 4106-66-5 | Mutagen |
| 507 | 6111-78-0 | Mutagen |
| 508 | 109-76-2 | Nonmutagen |
| 509 | 84-54-8 | Nonmutagen |
| 510 | 93-45-8 | Nonmutagen |
| 511 | 64188-65-4 | Mutagen |
| 512 | 149-57-5 | Nonmutagen |
| 513 | 760-23-6 | Nonmutagen |
| 514 | 659-70-1 | Nonmutagen |
| 515 | 56-40-6 | Nonmutagen |
| 516 | 6810-26-0 | Mutagen |
| 517 | 52517-34-7 | Mutagen |
| 518 | 479-50-5 | Mutagen |
| 519 | 21247-98-3 | Mutagen |
| 520 | 459-56-3 | Nonmutagen |
| 521 | 198-55-0 | Mutagen |
| 522 | 112-56-1 | Nonmutagen |
| 523 | 95896-78-9 | Mutagen |
| 524 | 17796-82-6 | Nonmutagen |
| 525 | 137-05-3 | Mutagen |
| 526 | 28911-01-5 | Nonmutagen |
| 527 | 2746-81-8 | Nonmutagen |
| 528 | 18463-85-9 | Mutagen |
| 529 | 86-50-0 | Mutagen |
| 530 | 92134-93-5 | Mutagen |
| 531 | 606-31-5 | Mutagen |
| 532 | 54755-20-3 | Mutagen |
| 533 | 66-56-8 | Mutagen |
| 534 | 118244-44-3 | Nonmutagen |
| 535 | 20426-12-4 | Nonmutagen |
| 536 | 31335-69-0 | Nonmutagen |
| 537 | 577-33-3 | Mutagen |
| 538 | 121-73-3 | Nonmutagen |
| 539 | 93673-39-3 | Mutagen |
| 540 | 146-22-5 | Nonmutagen |
| 541 | 1622-62-4 | Mutagen |
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| 543 | 02-02-3680 | Nonmutagen |
| 544 | 108-11-2 | Nonmutagen |
| 545 | 139953-78-9 | Mutagen |
| 546 | 104-55-2 | Nonmutagen |
| 547 | 86803-19-2 | Mutagen |
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| 549 | 05-07-2052 | Nonmutagen |
| 550 | 141-86-6 | Mutagen |
| 551 | 37962-27-9 | Mutagen |
| 552 | 771-29-9 | Mutagen |
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| 554 | 58-55-9 | Nonmutagen |
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| 556 | 107-31-3 | Nonmutagen |
| 557 | 619-23-8 | Mutagen |
| 558 | 546-88-3 | Mutagen |
| 559 | 112022-07-8 | Mutagen |
| 560 | 144-62-7 | Nonmutagen |
| 561 | 142713-63-1 | Mutagen |
| 562 | 120209-97-4 | Mutagen |
| 563 | 67-72-1 | Nonmutagen |
| 564 | 5447-11-0 | Nonmutagen |
| 565 | 120302-30-9 | Mutagen |
| 566 | 97-56-3 | Mutagen |
| 567 | 82-28-0 | Mutagen |
| 568 | 112-92-5 | Nonmutagen |
| 569 | 159092-72-5 | Mutagen |
| 570 | 91-19-0 | Mutagen |
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| 572 | 64894-89-9 | Mutagen |
| 573 | 35142-05-3 | Mutagen |
| 574 | 23696-28-8 | Mutagen |
| 575 | 759-94-4 | Nonmutagen |
| 576 | 3602-55-9 | Mutagen |
| 577 | 6237-22-5 | Mutagen |
| 578 | 114882-46-1 | Mutagen |
| 579 | 55302-96-0 | Nonmutagen |
| 580 | 2085-88-3 | Mutagen |
| 581 | 75-07-0 | Nonmutagen |
| 582 | 148193-31-1 | Mutagen |
| 583 | 2154-67-8 | Nonmutagen |
| 584 | 497-19-8 | Nonmutagen |
| 585 | 96563-06-3 | Mutagen |
| 586 | 86470-99-7 | Mutagen |
| 587 | 2984-50-1 | Nonmutagen |
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| 589 | 113779-16-1 | Mutagen |
| 590 | 138542-40-2 | Mutagen |
| 591 | 99-52-5 | Mutagen |
| 592 | 84-24-2 | Nonmutagen |
| 593 | 104-91-6 | Mutagen |
| 594 | 53473-85-1 | Mutagen |
| 595 | 93-15-2 | Nonmutagen |
| 596 | 932-97-8 | Mutagen |
| 597 | 26444-49-5 | Nonmutagen |
| 598 | 6628-97-3 | Mutagen |
| 599 | 1836-77-7 | Nonmutagen |
| 600 | 523-50-2 | Nonmutagen |
| 601 | 2478-38-8 | Nonmutagen |
| 602 | 109143-16-0 | Mutagen |
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| 604 | 13395-02-3 | Mutagen |
| 605 | 21362-69-6 | Nonmutagen |
| 606 | 7227-92-1 | Mutagen |
| 607 | 194-69-4 | Mutagen |
| 608 | 143-16-8 | Nonmutagen |
| 609 | 2872-48-2 | Mutagen |
| 610 | 6264-66-0 | Mutagen |
| 611 | 3268-49-3 | Nonmutagen |
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| 613 | 514-78-3 | Nonmutagen |
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| 615 | 13365-37-2 | Mutagen |
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| 634 | 98151-91-8 | Mutagen |
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| 699 | 215-62-3 | Mutagen |
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| 715 | 88847-89-6 | Nonmutagen |
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| 727 | 366-18-7 | Mutagen |
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| 780 | 557-11-9 | Mutagen |
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| 792 | 109-77-3 | Nonmutagen |
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| 794 | 93-46-9 | Mutagen |
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| 797 | 384-22-5 | Nonmutagen |
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| 1052 | 42978-43-8 | Mutagen |
| 1053 | 117-79-3 | Mutagen |
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| 1059 | 1904-98-9 | Nonmutagen |
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| 1066 | 20927-95-1 | Mutagen |
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| 1069 | 119-75-5 | Nonmutagen |
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| 1076 | 152-20-5 | Nonmutagen |
| 1077 | 3648-20-2 | Nonmutagen |
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| 1079 | 17241-59-7 | Nonmutagen |
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| 1095 | 999-55-3 | Nonmutagen |
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| 1107 | 461-58-5 | Mutagen |
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| 1111 | 74-95-3 | Mutagen |
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| 1132 | 1162-65-8 | Mutagen |
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| 1138 | 496-14-0 | Mutagen |
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| 1142 | 130-26-7 | Nonmutagen |
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| 1147 | 963-89-3 | Mutagen |
| 1148 | 610-48-0 | Nonmutagen |
| 1149 | 149-29-1 | Nonmutagen |
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| 1154 | 2358-84-1 | Nonmutagen |
| 1155 | 123-05-7 | Nonmutagen |
| 1156 | 15176-29-1 | Nonmutagen |
| 1157 | 58-93-5 | Nonmutagen |
| 1158 | 89-83-8 | Nonmutagen |
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| 1167 | 100-52-7 | Nonmutagen |
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| 1169 | 20020-02-4 | Nonmutagen |
| 1170 | 151378-34-6 | Mutagen |
| 1171 | 2403-28-3 | Nonmutagen |
| 1172 | 626-16-4 | Nonmutagen |
| 1173 | 542-85-8 | Nonmutagen |
| 1174 | 3114-70-3 | Nonmutagen |
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| 1185 | 75464-11-8 | Mutagen |
| 1186 | 66267-19-4 | Mutagen |
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| 1196 | 1768-31-6 | Mutagen |
| 1197 | 153954-29-1 | Mutagen |
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| 1202 | 3268-87-9 | Nonmutagen |
| 1203 | 82486-82-6 | Mutagen |
| 1204 | 617-35-6 | Nonmutagen |
| 1205 | 683-51-2 | Mutagen |
| 1206 | 111-84-2 | Nonmutagen |
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| 1214 | 95-68-1 | Mutagen |
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| 1223 | 2212-67-1 | Nonmutagen |
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| 1551 | 78411-56-0 | Mutagen |
| 1552 | 55256-49-0 | Nonmutagen |
| 1553 | 68247-85-8 | Mutagen |
| 1554 | 108-09-8 | Nonmutagen |
| 1555 | 13177-25-8 | Mutagen |
| 1556 | 3375-84-6 | Nonmutagen |
| 1557 | 6850-22-2 | Mutagen |
| 1558 | 555-84-0 | Mutagen |
| 1559 | 88-44-8 | Nonmutagen |
| 1560 | 5343-65-7 | Nonmutagen |
| 1561 | 86853-97-6 | Mutagen |
| 1562 | 84-88-8 | Mutagen |
| 1563 | 51-17-2 | Nonmutagen |
| 1564 | 106-30-9 | Nonmutagen |
| 1565 | 529-49-7 | Mutagen |
| 1566 | 64091-91-4 | Mutagen |
| 1567 | 66-71-7 | Nonmutagen |
| 1568 | 3351-30-2 | Mutagen |
| 1569 | 759-73-9 | Mutagen |
| 1570 | 17309-86-3 | Mutagen |
| 1571 | 32588-76-4 | Nonmutagen |
| 1572 | 03-05-2719 | Nonmutagen |
| 1573 | 620-22-4 | Nonmutagen |
| 1574 | 530-50-7 | Nonmutagen |
| 1575 | 1030-27-9 | Nonmutagen |
| 1576 | 13394-86-0 | Mutagen |
| 1577 | 9003-39-8 | Nonmutagen |
| 1578 | 148193-29-7 | Mutagen |
| 1579 | 29761-21-5 | Nonmutagen |
| 1580 | 16169-16-7 | Mutagen |
| 1581 | 25917-90-2 | Mutagen |
| 1582 | 98-51-1 | Nonmutagen |
| 1583 | 47165-04-8 | Nonmutagen |
| 1584 | 3475-63-6 | Mutagen |
| 1585 | 14129-84-1 | Mutagen |
| 1586 | 4376-20-9 | Nonmutagen |
| 1587 | 108-45-2 | Mutagen |
| 1588 | 51787-42-9 | Mutagen |
| 1589 | 57470-78-7 | Nonmutagen |
| 1590 | 91575-28-9 | Mutagen |
| 1591 | 2437-56-1 | Nonmutagen |
| 1592 | 102-08-9 | Nonmutagen |
| 1593 | 60516-11-2 | Mutagen |
| 1594 | 19881-18-6 | Mutagen |
| 1595 | 01-12-3077 | Mutagen |
| 1596 | 83053-57-0 | Nonmutagen |
| 1597 | 97136-66-8 | Mutagen |
| 1598 | 120812-51-3 | Mutagen |
| 1599 | 623-17-6 | Mutagen |
| 1600 | 13360-61-7 | Nonmutagen |
| 1601 | 96-91-3 | Mutagen |
| 1602 | 88-99-3 | Nonmutagen |
| 1603 | 81-63-0 | Mutagen |
| 1604 | 1192-62-7 | Mutagen |
| 1605 | 684-93-5 | Mutagen |
| 1606 | 202-98-2 | Mutagen |
| 1607 | 104-04-1 | Nonmutagen |
| 1608 | 71400-34-5 | Mutagen |
| 1609 | 56602-33-6 | Nonmutagen |
| 1610 | 126-98-7 | Nonmutagen |
| 1611 | 67-21-0 | Nonmutagen |
| 1612 | 1596-84-5 | Nonmutagen |
| 1613 | 104775-36-2 | Nonmutagen |
| 1614 | 88-14-2 | Nonmutagen |
| 1615 | 84-58-2 | Nonmutagen |
| 1616 | 52101-40-3 | Mutagen |
| 1617 | 529-19-1 | Nonmutagen |
| 1618 | 58430-01-6 | Mutagen |
| 1619 | 2782-91-4 | Nonmutagen |
| 1620 | 109875-50-5 | Mutagen |
| 1621 | 5221-17-0 | Mutagen |
| 1622 | 602-60-8 | Mutagen |
| 1623 | 92-69-3 | Mutagen |
| 1624 | 695-99-8 | Nonmutagen |
| 1625 | 122-57-6 | Mutagen |
| 1626 | 16757-80-5 | Mutagen |
| 1627 | 27758-60-7 | Mutagen |
| 1628 | 104-40-5 | Nonmutagen |
| 1629 | 14667-55-1 | Nonmutagen |
| 1630 | 823-86-9 | Nonmutagen |
| 1631 | 79455-30-4 | Nonmutagen |
| 1632 | 606-35-9 | Mutagen |
| 1633 | 316-49-4 | Mutagen |
| 1634 | 125-33-7 | Mutagen |
| 1635 | 105-39-5 | Nonmutagen |
| 1636 | 583-78-8 | Nonmutagen |
| 1637 | 25082-33-1 | Mutagen |
| 1638 | 1120-71-4 | Mutagen |
| 1639 | 4543-63-9 | Mutagen |
| 1640 | 74339-99-4 | Mutagen |
| 1641 | 55256-55-8 | Mutagen |
| 1642 | 13177-31-6 | Mutagen |
| 1643 | 111901-39-4 | Mutagen |
| 1644 | 580-17-6 | Mutagen |
| 1645 | 112965-21-6 | Nonmutagen |
| 1646 | 2498-76-2 | Mutagen |
| 1647 | 5910-89-4 | Nonmutagen |
| 1648 | 97-41-6 | Nonmutagen |
| 1649 | 604-75-1 | Nonmutagen |
| 1650 | 74-97-5 | Mutagen |
| 1651 | 3083-23-6 | Mutagen |
| 1652 | 107-35-7 | Nonmutagen |
| 1653 | 23491-44-3 | Nonmutagen |
| 1654 | 2902-96-7 | Nonmutagen |
| 1655 | 57775-29-8 | Nonmutagen |
| 1656 | 818-61-1 | Nonmutagen |
| 1657 | 2160-93-2 | Nonmutagen |
| 1658 | 64431-93-2 | Nonmutagen |
| 1659 | 528-75-6 | Mutagen |
| 1660 | 71-36-3 | Nonmutagen |
| 1661 | 482-44-0 | Mutagen |
| 1662 | 36536-46-6 | Mutagen |
| 1663 | 478-08-0 | Mutagen |
| 1664 | 159092-76-9 | Mutagen |
| 1665 | 24140-30-5 | Mutagen |
| 1666 | 120-12-7 | Mutagen |
| 1667 | 1421-63-2 | Mutagen |
| 1668 | 155798-37-1 | Mutagen |
| 1669 | 77191-36-7 | Nonmutagen |
| 1670 | 104485-01-0 | Nonmutagen |
| 1671 | 4463-22-3 | Mutagen |
| 1672 | 537-92-8 | Nonmutagen |
| 1673 | 96918-15-9 | Mutagen |
| 1674 | 125974-08-5 | Mutagen |
| 1675 | 7364-25-2 | Nonmutagen |
| 1676 | 93535-04-7 | Mutagen |
| 1677 | 41934-47-8 | Nonmutagen |
| 1678 | 535-11-5 | Mutagen |
| 1679 | 148193-35-5 | Mutagen |
| 1680 | 5836-85-1 | Mutagen |
| 1681 | 135086-94-1 | Mutagen |
| 1682 | 22008-60-2 | Nonmutagen |
| 1683 | 96346-61-1 | Nonmutagen |
| 1684 | 1456-28-6 | Mutagen |
| 1685 | 3029-19-4 | Mutagen |
| 1686 | 146795-48-4 | Mutagen |
| 1687 | 26328-53-0 | Nonmutagen |
| 1688 | 129-44-2 | Mutagen |
| 1689 | 99-56-9 | Mutagen |
| 1690 | 119-47-1 | Nonmutagen |
| 1691 | 90243-66-6 | Nonmutagen |
| 1692 | 3070-86-8 | Nonmutagen |
| 1693 | 3060-89-7 | Nonmutagen |
| 1694 | 530-75-6 | Nonmutagen |
| 1695 | 25155-23-1 | Nonmutagen |
| 1696 | 585-08-0 | Mutagen |
| 1697 | 63390-12-5 | Mutagen |
| 1698 | 62613-82-5 | Nonmutagen |
| 1699 | 4698-96-8 | Mutagen |
| 1700 | 13889-92-4 | Mutagen |
| 1701 | 2212-99-9 | Mutagen |
| 1702 | 62-55-5 | Nonmutagen |
| 1703 | 13925-00-3 | Nonmutagen |
| 1704 | 7132-67-4 | Mutagen |
| 1705 | 6375-16-2 | Mutagen |
| 1706 | 84174-21-0 | Mutagen |
| 1707 | 65002-17-7 | Nonmutagen |
| 1708 | 5802-60-8 | Nonmutagen |
| 1709 | 114607-46-4 | Nonmutagen |
| 1710 | 839-90-7 | Nonmutagen |
| 1711 | 106-91-2 | Mutagen |
| 1712 | 5989-27-5 | Nonmutagen |
| 1713 | 84434-42-4 | Mutagen |
| 1714 | 82414-02-6 | Mutagen |
| 1715 | 10387-13-0 | Mutagen |
| 1716 | 82-68-8 | Nonmutagen |
| 1717 | 15625-89-5 | Mutagen |
| 1718 | 587-04-2 | Nonmutagen |
| 1719 | 91-59-8 | Mutagen |
| 1720 | 121-47-1 | Nonmutagen |
| 1721 | 543-67-9 | Mutagen |
| 1722 | 4648-33-3 | Mutagen |
| 1723 | 04-12-6377 | Mutagen |
| 1724 | 645-49-8 | Nonmutagen |
| 1725 | 85-44-9 | Nonmutagen |
| 1726 | 134-20-3 | Nonmutagen |
| 1727 | 114-26-1 | Mutagen |
| 1728 | 121808-62-6 | Nonmutagen |
| 1729 | 18691-97-9 | Nonmutagen |
| 1730 | 84-64-0 | Nonmutagen |
| 1731 | 133591-33-0 | Mutagen |
| 1732 | 109-86-4 | Nonmutagen |
| 1733 | 102-50-1 | Mutagen |
| 1734 | 3234-28-4 | Nonmutagen |
| 1735 | 205-99-2 | Mutagen |
| 1736 | 107-05-1 | Mutagen |
| 1737 | 16238-56-5 | Mutagen |
| 1738 | 96-31-1 | Nonmutagen |
| 1739 | 1785-51-9 | Mutagen |
| 1740 | 918-00-3 | Mutagen |
| 1741 | 528-45-0 | Mutagen |
| 1742 | 101-70-2 | Nonmutagen |
| 1743 | 20268-51-3 | Nonmutagen |
| 1744 | 524-89-0 | Mutagen |
| 1745 | 105596-43-8 | Mutagen |
| 1746 | 57564-91-7 | Mutagen |
| 1747 | 40277-05-2 | Mutagen |
| 1748 | 2516-93-0 | Nonmutagen |
| 1749 | 27093-62-5 | Mutagen |
| 1750 | 23250-39-7 | Mutagen |
| 1751 | 95-51-2 | Nonmutagen |
| 1752 | 91-95-2 | Mutagen |
| 1753 | 87-59-2 | Mutagen |
| 1754 | 39081-15-7 | Mutagen |
| 1755 | 109-01-3 | Nonmutagen |
| 1756 | 105-45-3 | Nonmutagen |
| 1757 | 126572-78-9 | Mutagen |
| 1758 | 136-35-6 | Mutagen |
| 1759 | 151-67-7 | Nonmutagen |
| 1760 | 145438-97-7 | Mutagen |
| 1761 | 75-83-2 | Nonmutagen |
| 1762 | 2453-44-3 | Nonmutagen |
| 1763 | 108-21-4 | Nonmutagen |
| 1764 | 39515-41-8 | Nonmutagen |
| 1765 | 13171-00-1 | Nonmutagen |
| 1766 | 116539-70-9 | Mutagen |
| 1767 | 24191-98-8 | Mutagen |
| 1768 | 6441-91-4 | Nonmutagen |
| 1769 | 290-37-9 | Nonmutagen |
| 1770 | 98-46-4 | Nonmutagen |
| 1771 | 06-04-2486 | Mutagen |
| 1772 | 554-14-3 | Nonmutagen |
| 1773 | 88266-67-5 | Mutagen |
| 1774 | 475-38-7 | Mutagen |
| 1775 | 74340-04-8 | Mutagen |
| 1776 | 484-29-7 | Mutagen |
| 1777 | 509-93-3 | Nonmutagen |
| 1778 | 88-75-5 | Nonmutagen |
| 1779 | 634-91-3 | Nonmutagen |
| 1780 | 90-30-2 | Nonmutagen |
| 1781 | 885-82-5 | Nonmutagen |
| 1782 | 35089-70-4 | Mutagen |
| 1783 | 110-21-4 | Nonmutagen |
| 1784 | 1528-74-1 | Mutagen |
| 1785 | 131-14-6 | Mutagen |
| 1786 | 121-17-5 | Nonmutagen |
| 1787 | 80214-83-1 | Nonmutagen |
| 1788 | 92433-40-4 | Mutagen |
| 1789 | 2481-94-9 | Nonmutagen |
| 1790 | 75-17-2 | Nonmutagen |
| 1791 | 211-91-6 | Mutagen |
| 1792 | 611-36-9 | Nonmutagen |
| 1793 | 13132-28-0 | Mutagen |
| 1794 | 1805-02-3 | Mutagen |
| 1795 | 140-31-8 | Nonmutagen |
| 1796 | 486-25-9 | Nonmutagen |
| 1797 | 120-37-6 | Mutagen |
| 1798 | 2322-45-4 | Nonmutagen |
| 1799 | 70951-83-6 | Mutagen |
| 1800 | 107673-65-4 | Mutagen |
| 1801 | 766-40-5 | Mutagen |
| 1802 | 3771-19-5 | Nonmutagen |
| 1803 | 22755-15-3 | Mutagen |
| 1804 | 89459-25-6 | Mutagen |
| 1805 | 710-25-8 | Mutagen |
| 1806 | 28860-95-9 | Mutagen |
| 1807 | 51483-39-7 | Mutagen |
| 1808 | 134-09-8 | Nonmutagen |
| 1809 | 79-94-7 | Nonmutagen |
| 1810 | 2381-40-0 | Mutagen |
| 1811 | 87-10-5 | Nonmutagen |
| 1812 | 603-35-0 | Nonmutagen |
| 1813 | 31688-71-8 | Mutagen |
| 1814 | 2461-15-6 | Mutagen |
| 1815 | 88741-68-8 | Mutagen |
| 1816 | 43210-67-9 | Nonmutagen |
| 1817 | 19686-73-8 | Mutagen |
| 1818 | 2213-00-5 | Mutagen |
| 1819 | 144280-50-2 | Mutagen |
| 1820 | 86-30-6 | Nonmutagen |
| 1821 | 01-08-2164 | Nonmutagen |
| 1822 | 109875-45-8 | Mutagen |
| 1823 | 87-29-6 | Nonmutagen |
| 1824 | 113163-24-9 | Mutagen |
| 1825 | 81593-13-7 | Mutagen |
| 1826 | 15980-15-1 | Nonmutagen |
| 1827 | 101-59-7 | Mutagen |
| 1828 | 106636-48-0 | Mutagen |
| 1829 | 113058-39-2 | Mutagen |
| 1830 | 614-47-1 | Nonmutagen |
| 1831 | 962-32-3 | Mutagen |
| 1832 | 71382-44-0 | Mutagen |
| 1833 | 56258-32-3 | Mutagen |
| 1834 | 645-12-5 | Mutagen |
| 1835 | 7195-43-9 | Mutagen |
| 1836 | 72273-04-2 | Mutagen |
| 1837 | 13088-34-1 | Mutagen |
| 1838 | 10353-98-7 | Mutagen |
| 1839 | 77314-23-9 | Mutagen |
| 1840 | 520-18-3 | Mutagen |
| 1841 | 28164-57-0 | Nonmutagen |
| 1842 | 3296-90-0 | Mutagen |
| 1843 | 116208-67-4 | Mutagen |
| 1844 | 4823-47-6 | Mutagen |
| 1845 | 102791-33-3 | Mutagen |
| 1846 | 89-25-8 | Nonmutagen |
| 1847 | 19727-83-4 | Mutagen |
| 1848 | 92279-99-7 | Mutagen |
| 1849 | 98-16-8 | Nonmutagen |
| 1850 | 107-11-9 | Nonmutagen |
| 1851 | 5709-67-1 | Mutagen |
| 1852 | 1169-60-4 | Mutagen |
| 1853 | 17526-17-9 | Mutagen |
| 1854 | 13177-26-9 | Mutagen |
| 1855 | 5598-13-0 | Nonmutagen |
| 1856 | 17070-45-0 | Mutagen |
| 1857 | 1222-05-5 | Nonmutagen |
| 1858 | 88-45-9 | Nonmutagen |
| 1859 | 51-18-3 | Mutagen |
| 1860 | 66552-77-0 | Mutagen |
| 1861 | 90-00-6 | Nonmutagen |
| 1862 | 123-68-2 | Nonmutagen |
| 1863 | 24400-01-9 | Mutagen |
| 1864 | 5679-89-0 | Nonmutagen |
| 1865 | 2517-98-8 | Mutagen |
| 1866 | 1875-48-5 | Nonmutagen |
| 1867 | 3351-31-3 | Mutagen |
| 1868 | 1122-62-9 | Nonmutagen |
| 1869 | 117760-92-6 | Mutagen |
| 1870 | 6795-16-0 | Nonmutagen |
| 1871 | 85721-33-1 | Mutagen |
| 1872 | 34256-82-1 | Nonmutagen |
| 1873 | 2210-79-9 | Mutagen |
| 1874 | 60-35-5 | Nonmutagen |
| 1875 | 122-88-3 | Nonmutagen |
| 1876 | 611-06-3 | Mutagen |
| 1877 | 90-19-7 | Mutagen |
| 1878 | 95-76-1 | Nonmutagen |
| 1879 | 626-60-8 | Nonmutagen |
| 1880 | 129-20-4 | Mutagen |
| 1881 | 461-72-3 | Nonmutagen |
| 1882 | 53693-66-6 | Mutagen |
| 1883 | 581-28-2 | Mutagen |
| 1884 | 89-61-2 | Mutagen |
| 1885 | 16169-17-8 | Mutagen |
| 1886 | 94-96-2 | Nonmutagen |
| 1887 | 63655-40-3 | Mutagen |
| 1888 | 101021-43-6 | Mutagen |
| 1889 | 56980-94-0 | Nonmutagen |
| 1890 | 59229-75-3 | Mutagen |
| 1891 | 91575-29-0 | Mutagen |
| 1892 | 134-81-6 | Nonmutagen |
| 1893 | 930-22-3 | Mutagen |
| 1894 | 224-53-3 | Mutagen |
| 1895 | 17831-71-9 | Nonmutagen |
| 1896 | 304-28-9 | Mutagen |
| 1897 | 78-84-2 | Nonmutagen |
| 1898 | 132742-03-1 | Mutagen |
| 1899 | 86-00-0 | Nonmutagen |
| 1900 | 93106-60-6 | Mutagen |
| 1901 | 934-73-6 | Nonmutagen |
| 1902 | 52278-77-0 | Nonmutagen |
| 1903 | 76-03-9 | Nonmutagen |
| 1904 | 612-22-6 | Nonmutagen |
| 1905 | 834-28-6 | Nonmutagen |
| 1906 | 28622-66-4 | Mutagen |
| 1907 | 493-52-7 | Mutagen |
| 1908 | 147-47-7 | Nonmutagen |
| 1909 | 120812-52-4 | Mutagen |
| 1910 | 2540-82-1 | Nonmutagen |
| 1911 | 81-64-1 | Mutagen |
| 1912 | 94-11-1 | Nonmutagen |
| 1913 | 110-46-3 | Mutagen |
| 1914 | 1120-36-1 | Nonmutagen |
| 1915 | 476-60-8 | Mutagen |
| 1916 | 491-92-9 | Mutagen |
| 1917 | 124-18-5 | Nonmutagen |
| 1918 | 1825-21-4 | Mutagen |
| 1919 | 33100-27-5 | Nonmutagen |
| 1920 | 5408-55-9 | Mutagen |
| 1921 | 85068-73-1 | Mutagen |
| 1922 | 1640-39-7 | Nonmutagen |
| 1923 | 475-80-9 | Mutagen |
| 1924 | 334-48-5 | Nonmutagen |
| 1925 | 123-38-6 | Nonmutagen |
| 1926 | 125579-40-0 | Nonmutagen |
| 1927 | 19780-11-1 | Nonmutagen |
| 1928 | 1629-58-9 | Mutagen |
| 1929 | 2206-89-5 | Mutagen |
| 1930 | 127072-60-0 | Mutagen |
| 1931 | 128-95-0 | Mutagen |
| 1932 | 83-79-4 | Nonmutagen |
| 1933 | 111070-55-4 | Mutagen |
| 1934 | 42135-22-8 | Mutagen |
| 1935 | 2940-63-8 | Nonmutagen |
| 1936 | 4016-14-2 | Mutagen |
| 1937 | 95-46-5 | Nonmutagen |
| 1938 | 16757-81-6 | Mutagen |
| 1939 | 71382-50-8 | Mutagen |
| 1940 | 59863-59-1 | Mutagen |
| 1941 | 54-85-3 | Mutagen |
| 1942 | 491-26-9 | Nonmutagen |
| 1943 | 92078-92-7 | Mutagen |
| 1944 | 90147-18-5 | Mutagen |
| 1945 | 10125-76-5 | Mutagen |
| 1946 | 56211-40-6 | Nonmutagen |
| 1947 | 54854-14-7 | Nonmutagen |
| 1948 | 70644-19-8 | Mutagen |
| 1949 | 13177-32-7 | Mutagen |
| 1950 | 129-09-9 | Nonmutagen |
| 1951 | 111901-41-8 | Nonmutagen |
| 1952 | 5845-67-0 | Nonmutagen |
| 1953 | 141691-41-0 | Mutagen |
| 1954 | 580-18-7 | Nonmutagen |
| 1955 | 6926-44-9 | Mutagen |
| 1956 | 2498-77-3 | Mutagen |
| 1957 | 88-51-7 | Mutagen |
| 1958 | 5116-24-5 | Mutagen |
| 1959 | 102-81-8 | Nonmutagen |
| 1960 | 213-46-7 | Mutagen |
| 1961 | 08-09-7673 | Nonmutagen |
| 1962 | 119914-60-2 | Nonmutagen |
| 1963 | 56-81-5 | Nonmutagen |
| 1964 | 16110-13-7 | Mutagen |
| 1965 | 193-39-5 | Mutagen |
| 1966 | 613-93-4 | Nonmutagen |
| 1967 | 07-01-2565 | Mutagen |
| 1968 | 578-54-1 | Nonmutagen |
| 1969 | 69527-46-4 | Mutagen |
| 1970 | 552-30-7 | Nonmutagen |
| 1971 | 19057-60-4 | Nonmutagen |
| 1972 | 91182-09-1 | Mutagen |
| 1973 | 76600-84-5 | Nonmutagen |
| 1974 | 110-17-8 | Nonmutagen |
| 1975 | 100-19-6 | Mutagen |
| 1976 | 6728-26-3 | Mutagen |
| 1977 | 146795-30-4 | Mutagen |
| 1978 | 105553-32-0 | Mutagen |
| 1979 | 932-83-2 | Mutagen |
| 1980 | 66-97-7 | Nonmutagen |
| 1981 | 95-82-9 | Nonmutagen |
| 1982 | 78914-74-6 | Mutagen |
| 1983 | 105-76-0 | Nonmutagen |
| 1984 | 17557-23-2 | Mutagen |
| 1985 | 62674-12-8 | Mutagen |
| 1986 | 148193-36-6 | Mutagen |
| 1987 | 55610-00-9 | Mutagen |
| 1988 | 99-57-0 | Mutagen |
| 1989 | 540-73-8 | Nonmutagen |
| 1990 | 363-03-1 | Nonmutagen |
| 1991 | 78-90-0 | Nonmutagen |
| 1992 | 23045-12-7 | Mutagen |
| 1993 | 1576-87-0 | Mutagen |
| 1994 | 1555-94-8 | Nonmutagen |
| 1995 | 32959-60-7 | Nonmutagen |
| 1996 | 82-50-8 | Mutagen |
| 1997 | 62-56-6 | Nonmutagen |
| 1998 | 60784-46-5 | Mutagen |
| 1999 | 84174-22-1 | Mutagen |
| 2000 | 623-24-5 | Nonmutagen |
| 2001 | 89873-24-5 | Mutagen |
| 2002 | 548-04-9 | Nonmutagen |
| 2003 | 89837-94-5 | Mutagen |
| 2004 | 106-92-3 | Mutagen |
| 2005 | 25834-80-4 | Mutagen |
| 2006 | 118745-15-6 | Mutagen |
| 2007 | 94730-48-0 | Nonmutagen |
| 2008 | 51-79-6 | Mutagen |
| 2009 | 473-90-5 | Nonmutagen |
| 2010 | 478-45-5 | Nonmutagen |
| 2011 | 17987-99-4 | Mutagen |
| 2012 | 371-40-4 | Mutagen |
| 2013 | 2319-96-2 | Mutagen |
| 2014 | 1822-51-1 | Nonmutagen |
| 2015 | 2449-49-2 | Nonmutagen |
| 2016 | 127045-41-4 | Nonmutagen |
| 2017 | 836-30-6 | Nonmutagen |
| 2018 | 94-36-0 | Nonmutagen |
| 2019 | 115066-03-0 | Nonmutagen |
| 2020 | 22204-53-1 | Nonmutagen |
| 2021 | 91540-30-6 | Mutagen |
| 2022 | 621-64-7 | Mutagen |
| 2023 | 486-56-6 | Nonmutagen |
| 2024 | 25152-84-5 | Nonmutagen |
| 2025 | 16596-38-6 | Mutagen |
| 2026 | 480-19-3 | Nonmutagen |
| 2027 | 88-21-1 | Mutagen |
| 2028 | 36519-91-2 | Mutagen |
| 2029 | 1634-04-4 | Nonmutagen |
| 2030 | 84-65-1 | Mutagen |
| 2031 | 119-84-6 | Nonmutagen |
| 2032 | 67809-14-7 | Mutagen |
| 2033 | 127-00-4 | Mutagen |
| 2034 | 180913-77-3 | Mutagen |
| 2035 | 581-89-5 | Mutagen |
| 2036 | 1709-39-3 | Nonmutagen |
| 2037 | 17024-17-8 | Mutagen |
| 2038 | 67-47-0 | Mutagen |
| 2039 | 6344-63-4 | Mutagen |
| 2040 | 924-42-5 | Nonmutagen |
| 2041 | 5392-40-5 | Nonmutagen |
| 2042 | 20268-52-4 | Mutagen |
| 2043 | 93673-31-5 | Mutagen |
| 2044 | 7251-61-8 | Nonmutagen |
| 2045 | 60-11-7 | Mutagen |
| 2046 | 32954-58-8 | Nonmutagen |
| 2047 | 15254-64-5 | Mutagen |
| 2048 | 127-19-5 | Nonmutagen |
| 2049 | 3096-62-6 | Mutagen |
| 2050 | 109-02-4 | Nonmutagen |
| 2051 | 54-91-1 | Mutagen |
| 2052 | 108-22-5 | Nonmutagen |
| 2053 | 129-15-7 | Mutagen |
| 2054 | 141-97-9 | Nonmutagen |
| 2055 | 17057-98-6 | Mutagen |
| 2056 | 98-47-5 | Nonmutagen |
| 2057 | 74407-29-7 | Nonmutagen |
| 2058 | 602-01-7 | Mutagen |
| 2059 | 41267-76-9 | Mutagen |
| 2060 | 101-05-3 | Nonmutagen |
| 2061 | 1211-40-1 | Mutagen |
| 2062 | 3695-86-1 | Nonmutagen |
| 2063 | 78-79-5 | Nonmutagen |
| 2064 | 71-43-2 | Nonmutagen |
| 2065 | 67508-87-6 | Mutagen |
| 2066 | 5397-31-9 | Nonmutagen |
| 2067 | 82-39-3 | Mutagen |
| 2068 | 152-84-1 | Nonmutagen |
| 2069 | 100-25-4 | Mutagen |
| 2070 | 13024-49-2 | Mutagen |
| 2071 | 192-65-4 | Mutagen |
| 2072 | 23564-05-8 | Mutagen |
| 2073 | 97672-08-7 | Mutagen |
| 2074 | 3958-57-4 | Nonmutagen |
| 2075 | 104145-44-0 | Mutagen |
| 2076 | 736-31-2 | Mutagen |
| 2077 | 10312-83-1 | Mutagen |
| 2078 | 933-88-0 | Mutagen |
| 2079 | 6164-98-3 | Nonmutagen |
| 2080 | 01-12-3491 | Mutagen |
| 2081 | 86780-90-7 | Nonmutagen |
| 2082 | 4337-51-3 | Mutagen |
| 2083 | 88321-09-9 | Nonmutagen |
| 2084 | 2107-76-8 | Nonmutagen |
| 2085 | 3731-39-3 | Nonmutagen |
| 2086 | 5003-48-5 | Nonmutagen |
| 2087 | 107673-66-5 | Mutagen |
| 2088 | 185-70-6 | Nonmutagen |
| 2089 | 7083-63-8 | Mutagen |
| 2090 | 109-57-9 | Nonmutagen |
| 2091 | 83-44-3 | Nonmutagen |
| 2092 | 19077-98-6 | Nonmutagen |
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| 2094 | 158366-45-1 | Mutagen |
| 2095 | 55028-70-1 | Nonmutagen |
| 2096 | 98-83-9 | Nonmutagen |
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| 2099 | 475-75-2 | Mutagen |
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| 2101 | 143-27-1 | Nonmutagen |
| 2102 | 122-34-9 | Nonmutagen |
| 2103 | 152-18-1 | Nonmutagen |
| 2104 | 608-93-5 | Nonmutagen |
| 2105 | 2646-17-5 | Mutagen |
| 2106 | 619-89-6 | Mutagen |
| 2107 | 627-05-4 | Nonmutagen |
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| 2111 | 28361-96-8 | Mutagen |
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| 2114 | 98046-72-1 | Mutagen |
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| 2116 | 71382-45-1 | Mutagen |
| 2117 | 10353-99-8 | Mutagen |
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| 2143 | 132-86-5 | Mutagen |
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| 2205 | 95-47-6 | Nonmutagen |
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| 2207 | 16354-50-0 | Nonmutagen |
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| 2216 | 17526-24-8 | Mutagen |
| 2217 | 141691-42-1 | Mutagen |
| 2218 | 142457-04-3 | Mutagen |
| 2219 | 7779-16-0 | Nonmutagen |
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| 2222 | 123-75-1 | Nonmutagen |
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| 2238 | 120-14-9 | Nonmutagen |
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| 2249 | 64-17-5 | Nonmutagen |
| 2250 | 1340-08-5 | Nonmutagen |
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| 2252 | 122088-20-4 | Mutagen |
| 2253 | 135086-96-3 | Mutagen |
| 2254 | 952-97-6 | Mutagen |
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| 2260 | 128-66-5 | Nonmutagen |
| 2261 | 77-09-8 | Nonmutagen |
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| 2265 | 513-85-9 | Nonmutagen |
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| 2569 | 37151-16-9 | Mutagen |
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| 2576 | 171866-15-2 | Mutagen |
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| 2613 | 26266-68-2 | Nonmutagen |
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| 2615 | 842-07-9 | Mutagen |
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| 3119 | 78-94-4 | Mutagen |
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| 3580 | 57011-48-0 | Mutagen |
| 3581 | 367-25-9 | Mutagen |
| 3582 | 88193-04-8 | Mutagen |
| 3583 | 1210-35-1 | Nonmutagen |
| 3584 | 95-63-6 | Nonmutagen |
| 3585 | 3077-85-8 | Mutagen |
| 3586 | 501-53-1 | Nonmutagen |
| 3587 | 131-92-0 | Nonmutagen |
| 3588 | 30517-66-9 | Nonmutagen |
| 3589 | 89911-79-5 | Mutagen |
| 3590 | 16045-92-4 | Nonmutagen |
| 3591 | 2835-95-2 | Mutagen |
| 3592 | 591-12-8 | Nonmutagen |
| 3593 | 128714-76-1 | Mutagen |
| 3594 | 7203-90-9 | Mutagen |
| 3595 | 92758-43-5 | Mutagen |
| 3596 | 112022-10-3 | Mutagen |
| 3597 | 07-10-4752 | Nonmutagen |
| 3598 | 20930-10-3 | Mutagen |
| 3599 | 70249-46-6 | Nonmutagen |
| 3600 | 616-69-3 | Nonmutagen |
| 3601 | 114460-38-7 | Mutagen |
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| 3603 | 495-18-1 | Mutagen |
| 3604 | 1671-82-5 | Mutagen |
| 3605 | 123-91-1 | Nonmutagen |
| 3606 | 625-86-5 | Nonmutagen |
| 3607 | 2381-16-0 | Mutagen |
| 3608 | 99026-65-0 | Mutagen |
| 3609 | 91-22-5 | Mutagen |
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| 3619 | 2243-62-1 | Mutagen |
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| 3622 | 4406-41-1 | Nonmutagen |
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| 3624 | 146177-64-2 | Mutagen |
| 3625 | 119-65-3 | Nonmutagen |
| 3626 | 32534-81-9 | Nonmutagen |
| 3627 | 476-66-4 | Nonmutagen |
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| 3632 | 108-88-3 | Nonmutagen |
| 3633 | 1194-65-6 | Nonmutagen |
| 3634 | 3153-55-7 | Mutagen |
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| 3636 | 35212-22-7 | Nonmutagen |
| 3637 | 117929-12-1 | Mutagen |
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| 3639 | 86-42-0 | Nonmutagen |
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| 3647 | 80-05-7 | Nonmutagen |
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| 3649 | 19337-19-0 | Nonmutagen |
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| 3652 | 161697-02-5 | Mutagen |
| 3653 | 75-65-0 | Nonmutagen |
| 3654 | 3366-61-8 | Mutagen |
| 3655 | 130536-39-9 | Mutagen |
| 3656 | 52214-84-3 | Nonmutagen |
| 3657 | 922-63-4 | Mutagen |
| 3658 | 99-08-1 | Nonmutagen |
| 3659 | 7576-88-7 | Mutagen |
| 3660 | 108-03-2 | Nonmutagen |
| 3661 | 110-88-3 | Nonmutagen |
| 3662 | 37853-59-1 | Nonmutagen |
| 3663 | 39208-00-9 | Mutagen |
| 3664 | 16354-55-5 | Nonmutagen |
| 3665 | 141-78-6 | Nonmutagen |
| 3666 | 2784-94-3 | Mutagen |
| 3667 | 150-69-6 | Nonmutagen |
| 3668 | 86853-91-0 | Mutagen |
| 3669 | 116374-64-2 | Mutagen |
| 3670 | 122551-89-7 | Mutagen |
| 3671 | 97629-28-2 | Mutagen |
| 3672 | 129134-96-9 | Mutagen |
| 3673 | 619-15-8 | Mutagen |
| 3674 | 98033-25-1 | Mutagen |
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| 3677 | 92-93-3 | Mutagen |
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| 3679 | 106-43-4 | Nonmutagen |
| 3680 | 10213-75-9 | Nonmutagen |
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| 3685 | 141511-31-1 | Mutagen |
| 3686 | 146795-36-0 | Mutagen |
| 3687 | 5410-97-9 | Mutagen |
| 3688 | 104-83-6 | Nonmutagen |
| 3689 | 135-73-9 | Mutagen |
| 3690 | 541-59-3 | Mutagen |
| 3691 | 2832-40-8 | Mutagen |
| 3692 | 35282-68-9 | Mutagen |
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| 3700 | 1609-47-8 | Nonmutagen |
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| 3703 | 97-84-7 | Nonmutagen |
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| 3705 | 1025-15-6 | Nonmutagen |
| 3706 | 98601-00-4 | Mutagen |
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| 3717 | 89459-43-8 | Mutagen |
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| 3722 | 108-94-1 | Nonmutagen |
| 3723 | 61477-96-1 | Nonmutagen |
| 3724 | 105467-77-4 | Mutagen |
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| 3748 | 109-08-0 | Nonmutagen |
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| 3750 | 125-46-2 | Nonmutagen |
| 3751 | 141-84-4 | Nonmutagen |
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| 3753 | 520-36-5 | Nonmutagen |
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| 3755 | 113698-23-0 | Mutagen |
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| 3758 | 335-76-2 | Nonmutagen |
| 3759 | 112022-05-6 | Mutagen |
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| 3771 | 97-54-1 | Nonmutagen |
| 3772 | 2752-54-7 | Nonmutagen |
| 3773 | 71721-78-3 | Mutagen |
| 3774 | 136587-13-8 | Mutagen |
| 3775 | 51-36-5 | Nonmutagen |
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| 3786 | 85-02-9 | Mutagen |
| 3787 | 31438-22-9 | Mutagen |
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| 3790 | 1064-48-8 | Mutagen |
| 3791 | 121-54-0 | Nonmutagen |
| 3792 | 122-19-0 | Nonmutagen |
| 3793 | 1239-45-8 | Mutagen |
| 3794 | 124-64-1 | Nonmutagen |
| 3795 | 126-92-1 | Nonmutagen |
| 3796 | 135-20-6 | Mutagen |
| 3797 | 135-49-9 | Mutagen |
| 3798 | 137-09-7 | Mutagen |
| 3799 | 146-56-5 | Nonmutagen |
| 3800 | 15826-37-6 | Nonmutagen |
| 3801 | 1684-40-8 | Mutagen |
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| 3803 | 1936-15-8 | Nonmutagen |
| 3804 | 1937-37-7 | Mutagen |
| 3805 | 2045-52-5 | Nonmutagen |
| 3806 | 2216-51-5 | Nonmutagen |
| 3807 | 2390-59-2 | Mutagen |
| 3808 | 2429-73-4 | Mutagen |
| 3809 | 2429-82-5 | Mutagen |
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| 3812 | 01-05-2610 | Mutagen |
| 3813 | 09-11-2610 | Nonmutagen |
| 3814 | 2611-82-7 | Nonmutagen |
| 3815 | 298-59-9 | Nonmutagen |
| 3816 | 3087-16-9 | Nonmutagen |
| 3817 | 314-13-6 | Mutagen |
| 3818 | 32780-64-6 | Nonmutagen |
| 3819 | 3567-66-6 | Nonmutagen |
| 3820 | 3717-88-2 | Nonmutagen |
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| 3823 | 4213-45-0 | Mutagen |
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| 3826 | 05-04-5407 | Mutagen |
| 3827 | 569-61-9 | Mutagen |
| 3828 | 573-58-0 | Mutagen |
| 3829 | 58-33-3 | Nonmutagen |
| 3830 | 59-02-9 | Nonmutagen |
| 3831 | 590-46-5 | Nonmutagen |
| 3832 | 593-56-6 | Nonmutagen |
| 3833 | 61-73-4 | Mutagen |
| 3834 | 63-92-3 | Mutagen |
| 3835 | 632-99-5 | Mutagen |
| 3836 | 633-96-5 | Nonmutagen |
| 3837 | 65-61-2 | Mutagen |
| 3838 | 67-03-8 | Nonmutagen |
| 3839 | 69-05-6 | Mutagen |
| 3840 | 6959-47-3 | Mutagen |
| 3841 | 6959-48-4 | Mutagen |
| 3842 | 72-57-1 | Mutagen |
| 3843 | 81-88-9 | Mutagen |
| 3844 | 86-40-8 | Mutagen |
| 3845 | 92-31-9 | Mutagen |
| 3846 | 108-80-5 | Nonmutagen |
| 3847 | 1127-45-3 | Nonmutagen |
| 3848 | 115-02-6 | Mutagen |
| 3849 | 115-28-6 | Nonmutagen |
| 3850 | 119-39-1 | Nonmutagen |
| 3851 | 121-66-4 | Mutagen |
| 3852 | 1214-39-7 | Nonmutagen |
| 3853 | 1250-95-9 | Mutagen |
| 3854 | 130-01-8 | Nonmutagen |
| 3855 | 13010-08-7 | Mutagen |
| 3856 | 134-58-7 | Nonmutagen |
| 3857 | 137-66-6 | Nonmutagen |
| 3858 | 137-89-3 | Nonmutagen |
| 3859 | 1397-89-3 | Nonmutagen |
| 3860 | 1445-69-8 | Nonmutagen |
| 3861 | 148-82-3 | Mutagen |
| 3862 | 149-30-4 | Nonmutagen |
| 3863 | 149-32-6 | Nonmutagen |
| 3864 | 1686-14-2 | Nonmutagen |
| 3865 | 1747-60-0 | Mutagen |
| 3866 | 18172-33-3 | Nonmutagen |
| 3867 | 18883-66-4 | Mutagen |
| 3868 | 21259-20-1 | Nonmutagen |
| 3869 | 21794-01-4 | Nonmutagen |
| 3870 | 2270-40-8 | Nonmutagen |
| 3871 | 23255-69-8 | Nonmutagen |
| 3872 | 23282-20-4 | Nonmutagen |
| 3873 | 2349-67-9 | Nonmutagen |
| 3874 | 24815-24-5 | Nonmutagen |
| 3875 | 2550-75-6 | Nonmutagen |
| 3876 | 29975-16-4 | Nonmutagen |
| 3877 | 3048-64-4 | Nonmutagen |
| 3878 | 30516-87-1 | Mutagen |
| 3879 | 309-00-2 | Nonmutagen |
| 3880 | 315-22-0 | Nonmutagen |
| 3881 | 320-67-2 | Mutagen |
| 3882 | 327-97-9 | Nonmutagen |
| 3883 | 32795-84-9 | Mutagen |
| 3884 | 33089-61-1 | Nonmutagen |
| 3885 | 33419-42-0 | Nonmutagen |
| 3886 | 34807-41-5 | Nonmutagen |
| 3887 | 3682-19-7 | Mutagen |
| 3888 | 3868-31-3 | Nonmutagen |
| 3889 | 38966-21-1 | Nonmutagen |
| 3890 | 4245-76-5 | Nonmutagen |
| 3891 | 4245-77-6 | Mutagen |
| 3892 | 427-51-0 | Nonmutagen |
| 3893 | 04-03-4342 | Mutagen |
| 3894 | 03-03-4345 | Nonmutagen |
| 3895 | 461-89-2 | Mutagen |
| 3896 | 470-82-6 | Nonmutagen |
| 3897 | 471-80-7 | Nonmutagen |
| 3898 | 477-30-5 | Nonmutagen |
| 3899 | 481-49-2 | Mutagen |
| 3900 | 488-41-5 | Mutagen |
| 3901 | 50-07-7 | Mutagen |
| 3902 | 50-24-8 | Nonmutagen |
| 3903 | 50-27-1 | Nonmutagen |
| 3904 | 50-28-2 | Nonmutagen |
| 3905 | 50-44-2 | Mutagen |
| 3906 | 50-55-5 | Nonmutagen |
| 3907 | 50-76-0 | Nonmutagen |
| 3908 | 50-89-5 | Nonmutagen |
| 3909 | 51-21-8 | Nonmutagen |
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| 3912 | 51481-10-8 | Nonmutagen |
| 3913 | 517-28-2 | Nonmutagen |
| 3914 | 518-28-5 | Nonmutagen |
| 3915 | 518-34-3 | Mutagen |
| 3916 | 518-75-2 | Nonmutagen |
| 3917 | 520-26-3 | Nonmutagen |
| 3918 | 521-31-3 | Nonmutagen |
| 3919 | 53-43-0 | Nonmutagen |
| 3920 | 54-11-5 | Nonmutagen |
| 3921 | 54-42-2 | Nonmutagen |
| 3922 | 546-80-5 | Nonmutagen |
| 3923 | 555-30-6 | Nonmutagen |
| 3924 | 56-04-2 | Nonmutagen |
| 3925 | 56-86-0 | Nonmutagen |
| 3926 | 57-63-6 | Nonmutagen |
| 3927 | 57-83-0 | Nonmutagen |
| 3928 | 574-25-4 | Mutagen |
| 3929 | 58-61-7 | Nonmutagen |
| 3930 | 58-85-5 | Nonmutagen |
| 3931 | 58-94-6 | Nonmutagen |
| 3932 | 583-39-1 | Nonmutagen |
| 3933 | 59-14-3 | Nonmutagen |
| 3934 | 59-30-3 | Nonmutagen |
| 3935 | 59-92-7 | Mutagen |
| 3936 | 613-92-3 | Mutagen |
| 3937 | 616-91-1 | Mutagen |
| 3938 | 6219-89-2 | Mutagen |
| 3939 | 6285-57-0 | Mutagen |
| 3940 | 636-26-0 | Nonmutagen |
| 3941 | 6379-69-7 | Nonmutagen |
| 3942 | 67-97-0 | Nonmutagen |
| 3943 | 673-06-3 | Nonmutagen |
| 3944 | 68-22-4 | Nonmutagen |
| 3945 | 68-23-5 | Nonmutagen |
| 3946 | 70-00-8 | Mutagen |
| 3947 | 70-25-7 | Mutagen |
| 3948 | 700-02-7 | Mutagen |
| 3949 | 7059-24-7 | Nonmutagen |
| 3950 | 71-58-9 | Nonmutagen |
| 3951 | 73-03-0 | Mutagen |
| 3952 | 77-06-5 | Nonmutagen |
| 3953 | 77-73-6 | Nonmutagen |
| 3954 | 80-56-8 | Nonmutagen |
| 3955 | 80-78-4 | Nonmutagen |
| 3956 | 81-25-4 | Nonmutagen |
| 3957 | 87-33-2 | Nonmutagen |
| 3958 | 87-44-5 | Nonmutagen |
| 3959 | 89-65-6 | Nonmutagen |
| 3960 | 932-53-6 | Nonmutagen |
| 3961 | 951-78-0 | Nonmutagen |
| 3962 | 958-09-8 | Nonmutagen |
| 3963 | 96-50-4 | Mutagen |
| 3964 | 100-11-8 | Mutagen |
| 3965 | 105-54-4 | Nonmutagen |
| 3966 | 107-13-1 | Mutagen |
| 3967 | 1122-54-9 | Nonmutagen |
| 3968 | 2402-78-0 | Nonmutagen |
| 3969 | 311-45-5 | Mutagen |
| 3970 | 57-55-6 | Nonmutagen |
| 3971 | 78-83-1 | Nonmutagen |
| 3972 | 80-71-7 | Nonmutagen |
| 3973 | 90-33-5 | Nonmutagen |
| 3974 | 91-66-7 | Nonmutagen |
| 3975 | 96-12-8 | Mutagen |
| 3976 | 97-88-1 | Nonmutagen |
| 3977 | 107-06-2 | Mutagen |
| 3978 | 1146-04-9 | Mutagen |
| 3979 | 1149-99-1 | Mutagen |
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| 3983 | 13010-10-1 | Mutagen |
| 3984 | 13849-08-6 | Mutagen |
| 3985 | 1456-55-9 | Nonmutagen |
| 3986 | 1605-06-7 | Mutagen |
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| 3988 | 1947-37-1 | Nonmutagen |
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| 3990 | 203-33-8 | Mutagen |
| 3991 | 20830-81-3 | Mutagen |
| 3992 | 21313-86-0 | Mutagen |
| 3993 | 2163-68-0 | Nonmutagen |
| 3994 | 21794-55-8 | Mutagen |
| 3995 | 21884-44-6 | Nonmutagen |
| 3996 | 22897-08-1 | Mutagen |
| 3997 | 23537-16-8 | Nonmutagen |
| 3998 | 23815-63-6 | Mutagen |
| 3999 | 27046-19-1 | Mutagen |
| 4000 | 06-05-2958 | Nonmutagen |
| 4001 | 29767-20-2 | Mutagen |
| 4002 | 299-75-2 | Mutagen |
| 4003 | 01-01-3054 | Nonmutagen |
| 4004 | 3081-61-6 | Nonmutagen |
| 4005 | 320-51-4 | Nonmutagen |
| 4006 | 33069-62-4 | Nonmutagen |
| 4007 | 3311-98-6 | Mutagen |
| 4008 | 3414-62-8 | Mutagen |
| 4009 | 352-11-4 | Nonmutagen |
| 4010 | 09-10-3546 | Nonmutagen |
| 4011 | 362-74-3 | Nonmutagen |
| 4012 | 372-47-4 | Nonmutagen |
| 4013 | 3836-23-5 | Nonmutagen |
| 4014 | 40297-54-9 | Nonmutagen |
| 4015 | 43000-65-3 | Mutagen |
| 4016 | 4494-26-2 | Nonmutagen |
| 4017 | 480-81-9 | Mutagen |
| 4018 | 491-36-1 | Nonmutagen |
| 4019 | 4914-30-1 | Nonmutagen |
| 4020 | 50-63-5 | Mutagen |
| 4021 | 514-10-3 | Nonmutagen |
| 4022 | 535-83-1 | Nonmutagen |
| 4023 | 5418-93-9 | Nonmutagen |
| 4024 | 5461-85-8 | Mutagen |
| 4025 | 548-42-5 | Mutagen |
| 4026 | 569-26-6 | Mutagen |
| 4027 | 57-47-6 | Nonmutagen |
| 4028 | 570-74-1 | Nonmutagen |
| 4029 | 58-19-5 | Nonmutagen |
| 4030 | 598-57-2 | Nonmutagen |
| 4031 | 60-57-1 | Nonmutagen |
| 4032 | 60254-83-3 | Nonmutagen |
| 4033 | 604-35-3 | Nonmutagen |
| 4034 | 61-82-5 | Nonmutagen |
| 4035 | 611-53-0 | Nonmutagen |
| 4036 | 621-44-3 | Nonmutagen |
| 4037 | 6285-68-3 | Mutagen |
| 4038 | 63166-73-4 | Nonmutagen |
| 4039 | 64-86-8 | Nonmutagen |
| 4040 | 668-17-7 | Mutagen |
| 4041 | 67199-66-0 | Mutagen |
| 4042 | 68884-32-2 | Mutagen |
| 4043 | 69245-38-1 | Mutagen |
| 4044 | 70-18-8 | Mutagen |
| 4045 | 71-33-0 | Nonmutagen |
| 4046 | 7570-86-7 | Mutagen |
| 4047 | 79-92-5 | Nonmutagen |
| 4048 | 83-95-4 | Mutagen |
| 4049 | 86-54-4 | Mutagen |
| 4050 | 89925-00-8 | Mutagen |
| 4051 | 9002-92-0 | Nonmutagen |
| 4052 | 90597-22-1 | Nonmutagen |
| 4053 | 924-43-6 | Mutagen |

**Supplementary 2:** Molecular features used in current study **(**Page no. 92-155)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Name** | **Description** | **Block** |  |
| 1 | MW | molecular weight | Constitutional indices |  |
| 2 | AMW | average molecular weight | Constitutional indices |  |
| 3 | Sv | sum of atomic van der Waals volumes (scaled on Carbon atom) | Constitutional indices |  |
| 4 | Se | sum of atomic Sanderson electronegativities (scaled on Carbon atom) | Constitutional indices |  |
| 5 | Sp | sum of atomic polarizabilities (scaled on Carbon atom) | Constitutional indices |  |
| 6 | Si | sum of first ionization potentials (scaled on Carbon atom) | Constitutional indices |  |
| 7 | Mv | mean atomic van der Waals volume (scaled on Carbon atom) | Constitutional indices |  |
| 8 | Me | mean atomic Sanderson electronegativity (scaled on Carbon atom) | Constitutional indices |  |
| 9 | Mp | mean atomic polarizability (scaled on Carbon atom) | Constitutional indices |  |
| 10 | Mi | mean first ionization potential (scaled on Carbon atom) | Constitutional indices |  |
| 11 | nAT | number of atoms | Constitutional indices |  |
| 12 | nSK | number of non-H atoms | Constitutional indices |  |
| 13 | nBT | number of bonds | Constitutional indices |  |
| 14 | nBO | number of non-H bonds | Constitutional indices |  |
| 15 | nBM | number of multiple bonds | Constitutional indices |  |
| 16 | SCBO | sum of conventional bond orders (H-depleted) | Constitutional indices |  |
| 17 | RBN | number of rotatable bonds | Constitutional indices |  |
| 18 | RBF | rotatable bond fraction | Constitutional indices |  |
| 19 | nDB | number of double bonds | Constitutional indices |  |
| 20 | nTB | number of triple bonds | Constitutional indices |  |
| 21 | nAB | number of aromatic bonds | Constitutional indices |  |
| 22 | nH | number of Hydrogen atoms | Constitutional indices |  |
| 23 | nC | number of Carbon atoms | Constitutional indices |  |
| 24 | nN | number of Nitrogen atoms | Constitutional indices |  |
| 25 | nO | number of Oxygen atoms | Constitutional indices |  |
| 26 | nP | number of Phosphorous atoms | Constitutional indices |  |
| 27 | nS | number of Sulfur atoms | Constitutional indices |  |
| 28 | nF | number of Fluorine atoms | Constitutional indices |  |
| 29 | nCL | number of Chlorine atoms | Constitutional indices |  |
| 30 | nBR | number of Bromine atoms | Constitutional indices |  |
| 31 | nI | number of Iodine atoms | Constitutional indices |  |
| 32 | nX | number of halogen atoms | Constitutional indices |  |
| 33 | ARR | aromatic ratio | Ring descriptors |  |
| 34 | nCIC | number of rings (cyclomatic number) | Ring descriptors |  |
| 35 | nCIR | number of circuits | Ring descriptors |  |
| 36 | nR03 | number of 3-membered rings | Ring descriptors |  |
| 37 | nR04 | number of 4-membered rings | Ring descriptors |  |
| 38 | nR05 | number of 5-membered rings | Ring descriptors |  |
| 39 | nR06 | number of 6-membered rings | Ring descriptors |  |
| 40 | nR07 | number of 7-membered rings | Ring descriptors |  |
| 41 | nR08 | number of 8-membered rings | Ring descriptors |  |
| 42 | nR09 | number of 9-membered rings | Ring descriptors |  |
| 43 | nR10 | number of 10-membered rings | Ring descriptors |  |
| 44 | nR11 | number of 11-membered rings | Ring descriptors |  |
| 45 | nR12 | number of 12-membered rings | Ring descriptors |  |
| 46 | nBnz | number of benzene-like rings | Ring descriptors |  |
| 47 | ZM1 | first Zagreb index | Topological indices |  |
| 48 | ZM1V | first Zagreb index by valence vertex degrees | Topological indices |  |
| 49 | ZM2 | second Zagreb index | Topological indices |  |
| 50 | ZM2V | second Zagreb index by valence vertex degrees | Topological indices |  |
| 51 | Qindex | quadratic index | Topological indices |  |
| 52 | SNar | Narumi simple topological index (log function) | Topological indices |  |
| 53 | HNar | Narumi harmonic topological index | Topological indices |  |
| 54 | GNar | Narumi geometric topological index | Topological indices |  |
| 55 | Xt | total structure connectivity index | Topological indices |  |
| 56 | Dz | Pogliani index | Topological indices |  |
| 57 | Ram | ramification index | Topological indices |  |
| 58 | Pol | polarity number | Topological indices |  |
| 59 | LPRS | log of product of row sums (PRS) | Topological indices |  |
| 60 | MSD | mean square distance index (Balaban) | Topological indices |  |
| 61 | SPI | superpendentic index | Topological indices |  |
| 62 | PJI2 | 2D Petitjean shape index | Topological indices |  |
| 63 | VDA | average vertex distance degree | Topological indices |  |
| 64 | GMTI | Gutman Molecular Topological Index | Topological indices |  |
| 65 | GMTIV | Gutman Molecular Topological Index by valence vertex degrees | Topological indices |  |
| 66 | Xu | Xu index | Topological indices |  |
| 67 | W | Wiener Index | Topological indices |  |
| 68 | WA | mean Wiener index | Topological indices |  |
| 69 | SMTI | Schultz Molecular Topological Index (MTI) | Topological indices |  |
| 70 | SMTIV | Schultz Molecular Topological Index by valence vertex degrees | Topological indices |  |
| 71 | Har | Harary H index | Topological indices |  |
| 72 | Har2 | square reciprocal distance sum index | Topological indices |  |
| 73 | QW\_L | quasi-Wiener index (Kirchhoff number) from Laplace matrix | 2D matrix-based descriptors |  |
| 74 | TI1\_L | first Mohar index from Laplace matrix | 2D matrix-based descriptors |  |
| 75 | TI2\_L | second Mohar index from Laplace matrix | 2D matrix-based descriptors |  |
| 76 | STN\_L | spanning tree number (log function) from Laplace matrix | 2D matrix-based descriptors |  |
| 77 | NRS | number of ring systems | Ring descriptors |  |
| 78 | NNRS | normalized number of ring systems | Ring descriptors |  |
| 79 | w | detour index | Topological indices |  |
| 80 | ww | hyper-detour index | Topological indices |  |
| 81 | Rww | reciprocal hyper-detour index | Topological indices |  |
| 82 | D/D | distance/detour index | Topological indices |  |
| 83 | Wap | all-path Wiener index | Topological indices |  |
| 84 | WhetZ | Wiener-type index from Z weighted distance matrix (Barysz matrix) | Topological indices |  |
| 85 | Whetm | Wiener-type index from mass weighted distance matrix | Topological indices |  |
| 86 | Whetv | Wiener-type index from van der Waals weighted distance matrix | Topological indices |  |
| 87 | Whete | Wiener-type index from electronegativity weighted distance matrix | Topological indices |  |
| 88 | Whetp | Wiener-type index from polarizability weighted distance matrix | Topological indices |  |
| 89 | ECC | eccentricity | Topological indices |  |
| 90 | AECC | average eccentricity | Topological indices |  |
| 91 | DECC | eccentric | Topological indices |  |
| 92 | J | Balaban-like index from adjacency matrix | 2D matrix-based descriptors |  |
| 93 | BLI | Kier benzene-likeliness index | Topological indices |  |
| 94 | JhetZ | Balaban-type index from Z weighted distance matrix (Barysz matrix) | Topological indices |  |
| 95 | Jhetm | Balaban-type index from mass weighted distance matrix | Topological indices |  |
| 96 | Jhetv | Balaban-type index from van der Waals weighted distance matrix | Topological indices |  |
| 97 | Jhete | Balaban-type index from electronegativity weighted distance matrix | Topological indices |  |
| 98 | Jhetp | Balaban-type index from polarizability weighted distance matrix | Topological indices |  |
| 99 | MAXDN | maximal electrotopological negative variation | Topological indices |  |
| 100 | MAXDP | maximal electrotopological positive variation | Topological indices |  |
| 101 | DELS | molecular electrotopological variation | Topological indices |  |
| 102 | TIE | E-state topological parameter | Topological indices |  |
| 103 | S0K | Kier symmetry index | Topological indices |  |
| 104 | S1K | 1-path Kier alpha-modified shape index | Topological indices |  |
| 105 | S2K | 2-path Kier alpha-modified shape index | Topological indices |  |
| 106 | S3K | 3-path Kier alpha-modified shape index | Topological indices |  |
| 107 | PHI | Kier flexibility index | Topological indices |  |
| 108 | PW2 | path/walk 2 - Randic shape index | Topological indices |  |
| 109 | PW3 | path/walk 3 - Randic shape index | Topological indices |  |
| 110 | PW4 | path/walk 4 - Randic shape index | Topological indices |  |
| 111 | PW5 | path/walk 5 - Randic shape index | Topological indices |  |
| 112 | CSI | eccentric connectivity index | Topological indices |  |
| 113 | MDDD | mean distance degree deviation | Topological indices |  |
| 114 | UNIP | unipolarity | Topological indices |  |
| 115 | CENT | centralization | Topological indices |  |
| 116 | VAR | variation | Topological indices |  |
| 117 | BAC | Balaban centric index | Topological indices |  |
| 118 | Lop | Lopping centric index | Topological indices |  |
| 119 | ICR | radial centric information index | Topological indices |  |
| 120 | D/Dr03 | distance/detour ring index of order 3 | Topological indices |  |
| 121 | D/Dr04 | distance/detour ring index of order 4 | Topological indices |  |
| 122 | D/Dr05 | distance/detour ring index of order 5 | Topological indices |  |
| 123 | D/Dr06 | distance/detour ring index of order 6 | Topological indices |  |
| 124 | D/Dr07 | distance/detour ring index of order 7 | Topological indices |  |
| 125 | D/Dr08 | distance/detour ring index of order 8 | Topological indices |  |
| 126 | D/Dr09 | distance/detour ring index of order 9 | Topological indices |  |
| 127 | D/Dr10 | distance/detour ring index of order 10 | Topological indices |  |
| 128 | D/Dr11 | distance/detour ring index of order 11 | Topological indices |  |
| 129 | D/Dr12 | distance/detour ring index of order 12 | Topological indices |  |
| 130 | T(N..N) | sum of topological distances between N..N | Topological indices |  |
| 131 | T(N..O) | sum of topological distances between N..O | Topological indices |  |
| 132 | T(N..S) | sum of topological distances between N..S | Topological indices |  |
| 133 | T(N..P) | sum of topological distances between N..P | Topological indices |  |
| 134 | T(N..F) | sum of topological distances between N..F | Topological indices |  |
| 135 | T(N..Cl) | sum of topological distances between N..Cl | Topological indices |  |
| 136 | T(N..Br) | sum of topological distances between N..Br | Topological indices |  |
| 137 | T(N..I) | sum of topological distances between N..I | Topological indices |  |
| 138 | T(O..O) | sum of topological distances between O..O | Topological indices |  |
| 139 | T(O..S) | sum of topological distances between O..S | Topological indices |  |
| 140 | T(O..P) | sum of topological distances between O..P | Topological indices |  |
| 141 | T(O..F) | sum of topological distances between O..F | Topological indices |  |
| 142 | T(O..Cl) | sum of topological distances between O..Cl | Topological indices |  |
| 143 | T(O..Br) | sum of topological distances between O..Br | Topological indices |  |
| 144 | T(O..I) | sum of topological distances between O..I | Topological indices |  |
| 145 | T(S..S) | sum of topological distances between S..S | Topological indices |  |
| 146 | T(S..P) | sum of topological distances between S..P | Topological indices |  |
| 147 | T(S..F) | sum of topological distances between S..F | Topological indices |  |
| 148 | T(S..Cl) | sum of topological distances between S..Cl | Topological indices |  |
| 149 | T(S..Br) | sum of topological distances between S..Br | Topological indices |  |
| 150 | T(P..P) | sum of topological distances between P..P | Topological indices |  |
| 151 | T(P..Cl) | sum of topological distances between P..Cl | Topological indices |  |
| 152 | T(P..Br) | sum of topological distances between P..Br | Topological indices |  |
| 153 | T(F..F) | sum of topological distances between F..F | Topological indices |  |
| 154 | T(F..Cl) | sum of topological distances between F..Cl | Topological indices |  |
| 155 | T(F..Br) | sum of topological distances between F..Br | Topological indices |  |
| 156 | T(Cl..Cl) | sum of topological distances between Cl..Cl | Topological indices |  |
| 157 | T(Cl..Br) | sum of topological distances between Cl..Br | Topological indices |  |
| 158 | T(Br..Br) | sum of topological distances between Br..Br | Topological indices |  |
| 159 | MWC01 | molecular walk count of order 1 | Walk and path counts |  |
| 160 | MWC02 | molecular walk count of order 2 | Walk and path counts |  |
| 161 | MWC03 | molecular walk count of order 3 | Walk and path counts |  |
| 162 | MWC04 | molecular walk count of order 4 | Walk and path counts |  |
| 163 | MWC05 | molecular walk count of order 5 | Walk and path counts |  |
| 164 | MWC06 | molecular walk count of order 6 | Walk and path counts |  |
| 165 | MWC07 | molecular walk count of order 7 | Walk and path counts |  |
| 166 | MWC08 | molecular walk count of order 8 | Walk and path counts |  |
| 167 | MWC09 | molecular walk count of order 9 | Walk and path counts |  |
| 168 | MWC10 | molecular walk count of order 10 | Walk and path counts |  |
| 169 | TWC | total walk count | Walk and path counts |  |
| 170 | SRW01 | self-returning walk count of order 2 | Walk and path counts |  |
| 171 | SRW02 | self-returning walk count of order 2 | Walk and path counts |  |
| 172 | SRW03 | self-returning walk count of order 3 | Walk and path counts |  |
| 173 | SRW04 | self-returning walk count of order 4 | Walk and path counts |  |
| 174 | SRW05 | self-returning walk count of order 5 | Walk and path counts |  |
| 175 | SRW06 | self-returning walk count of order 6 | Walk and path counts |  |
| 176 | SRW07 | self-returning walk count of order 7 | Walk and path counts |  |
| 177 | SRW08 | self-returning walk count of order 8 | Walk and path counts |  |
| 178 | SRW09 | self-returning walk count of order 9 | Walk and path counts |  |
| 179 | SRW10 | self-returning walk count of order 10 | Walk and path counts |  |
| 180 | MPC01 | molecular path count of order 1 (no. of non-H bonds) | Walk and path counts |  |
| 181 | MPC02 | molecular path count of order 2 (Gordon-Scantlebury index) | Walk and path counts |  |
| 182 | MPC03 | molecular path count of order 3 | Walk and path counts |  |
| 183 | MPC04 | molecular path count of order 4 | Walk and path counts |  |
| 184 | MPC05 | molecular path count of order 5 | Walk and path counts |  |
| 185 | MPC06 | molecular path count of order 6 | Walk and path counts |  |
| 186 | MPC07 | molecular path count of order 7 | Walk and path counts |  |
| 187 | MPC08 | molecular path count of order 8 | Walk and path counts |  |
| 188 | MPC09 | molecular path count of order 9 | Walk and path counts |  |
| 189 | MPC10 | molecular path count of order 10 | Walk and path counts |  |
| 190 | piPC01 | molecular multiple path count of order 1 | Walk and path counts |  |
| 191 | piPC02 | molecular multiple path count of order 2 | Walk and path counts |  |
| 192 | piPC03 | molecular multiple path count of order 3 | Walk and path counts |  |
| 193 | piPC04 | molecular multiple path count of order 4 | Walk and path counts |  |
| 194 | piPC05 | molecular multiple path count of order 5 | Walk and path counts |  |
| 195 | piPC06 | molecular multiple path count of order 6 | Walk and path counts |  |
| 196 | piPC07 | molecular multiple path count of order 7 | Walk and path counts |  |
| 197 | piPC08 | molecular multiple path count of order 8 | Walk and path counts |  |
| 198 | piPC09 | molecular multiple path count of order 9 | Walk and path counts |  |
| 199 | piPC10 | molecular multiple path count of order 10 | Walk and path counts |  |
| 200 | TPC | total path count | Walk and path counts |  |
| 201 | piID | conventional bond order ID number | Walk and path counts |  |
| 202 | PCR | ratio of multiple path count over path count | Walk and path counts |  |
| 203 | PCD | difference between multiple path count and path count | Walk and path counts |  |
| 204 | CID | Randic ID number | Walk and path counts |  |
| 205 | BID | Balaban ID number | Walk and path counts |  |
| 206 | X0 | connectivity index of order 0 | Connectivity indices |  |
| 207 | X1 | connectivity index of order 1 (Randic connectivity index) | Connectivity indices |  |
| 208 | X2 | connectivity index of order 2 | Connectivity indices |  |
| 209 | X3 | connectivity index of order 3 | Connectivity indices |  |
| 210 | X4 | connectivity index of order 4 | Connectivity indices |  |
| 211 | X5 | connectivity index of order 5 | Connectivity indices |  |
| 212 | X0A | average connectivity index of order 0 | Connectivity indices |  |
| 213 | X1A | average connectivity index of order 1 | Connectivity indices |  |
| 214 | X2A | average connectivity index of order 2 | Connectivity indices |  |
| 215 | X3A | average connectivity index of order 3 | Connectivity indices |  |
| 216 | X4A | average connectivity index of order 4 | Connectivity indices |  |
| 217 | X5A | average connectivity index of order 5 | Connectivity indices |  |
| 218 | X0v | valence connectivity index of order 0 | Connectivity indices |  |
| 219 | X1v | valence connectivity index of order 1 | Connectivity indices |  |
| 220 | X2v | valence connectivity index of order 2 | Connectivity indices |  |
| 221 | X3v | valence connectivity index of order 3 | Connectivity indices |  |
| 222 | X4v | valence connectivity index of order 4 | Connectivity indices |  |
| 223 | X5v | valence connectivity index of order 5 | Connectivity indices |  |
| 224 | X0Av | average valence connectivity index of order 0 | Connectivity indices |  |
| 225 | X1Av | average valence connectivity index of order 1 | Connectivity indices |  |
| 226 | X2Av | average valence connectivity index of order 2 | Connectivity indices |  |
| 227 | X3Av | average valence connectivity index of order 3 | Connectivity indices |  |
| 228 | X4Av | average valence connectivity index of order 4 | Connectivity indices |  |
| 229 | X5Av | average valence connectivity index of order 5 | Connectivity indices |  |
| 230 | X0sol | solvation connectivity index of order 0 | Connectivity indices |  |
| 231 | X1sol | solvation connectivity index of order 1 | Connectivity indices |  |
| 232 | X2sol | solvation connectivity index of order 2 | Connectivity indices |  |
| 233 | X3sol | solvation connectivity index of order 3 | Connectivity indices |  |
| 234 | X4sol | solvation connectivity index of order 4 | Connectivity indices |  |
| 235 | X5sol | solvation connectivity index of order 5 | Connectivity indices |  |
| 236 | XMOD | modified Randic index | Connectivity indices |  |
| 237 | RDCHI | reciprocal distance sum Randic-like index | Connectivity indices |  |
| 238 | RDSQ | reciprocal distance sum inverse Randic-like index | Connectivity indices |  |
| 239 | ISIZ | information index on molecular size | Information indices |  |
| 240 | IAC | total information index on atomic composition | Information indices |  |
| 241 | AAC | mean information index on atomic composition | Information indices |  |
| 242 | IDE | mean information content on the distance equality | Information indices |  |
| 243 | IDM | mean information content on the distance magnitude | Information indices |  |
| 244 | IDDE | mean information content on the distance degree equality | Information indices |  |
| 245 | IDDM | mean information content on the distance degree magnitude | Information indices |  |
| 246 | IDET | total information content on the distance equality | Information indices |  |
| 247 | IDMT | total information content on the distance magnitude | Information indices |  |
| 248 | IVDE | mean information content on the vertex degree equality | Information indices |  |
| 249 | IVDM | mean information content on the vertex degree magnitude | Information indices |  |
| 250 | HVcpx | graph vertex complexity index | Information indices |  |
| 251 | HDcpx | graph distance complexity index (log function) | Information indices |  |
| 252 | Uindex | Balaban U index | Information indices |  |
| 253 | Vindex | Balaban V index | Information indices |  |
| 254 | Xindex | Balaban X index | Information indices |  |
| 255 | Yindex | Balaban Y index | Information indices |  |
| 256 | IC0 | Information Content index (neighborhood symmetry of 0-order) | Information indices |  |
| 257 | TIC0 | Total Information Content index (neighborhood symmetry of 0-order) | Information indices |  |
| 258 | SIC0 | Structural Information Content index (neighborhood symmetry of 0-order) | Information indices |  |
| 259 | CIC0 | Complementary Information Content index (neighborhood symmetry of 0-order) | Information indices |  |
| 260 | BIC0 | Bond Information Content index (neighborhood symmetry of 0-order) | Information indices |  |
| 261 | IC1 | Information Content index (neighborhood symmetry of 1-order) | Information indices |  |
| 262 | TIC1 | Total Information Content index (neighborhood symmetry of 1-order) | Information indices |  |
| 263 | SIC1 | Structural Information Content index (neighborhood symmetry of 1-order) | Information indices |  |
| 264 | CIC1 | Complementary Information Content index (neighborhood symmetry of 1-order) | Information indices |  |
| 265 | BIC1 | Bond Information Content index (neighborhood symmetry of 1-order) | Information indices |  |
| 266 | IC2 | Information Content index (neighborhood symmetry of 2-order) | Information indices |  |
| 267 | TIC2 | Total Information Content index (neighborhood symmetry of 2-order) | Information indices |  |
| 268 | SIC2 | Structural Information Content index (neighborhood symmetry of 2-order) | Information indices |  |
| 269 | CIC2 | Complementary Information Content index (neighborhood symmetry of 2-order) | Information indices |  |
| 270 | BIC2 | Bond Information Content index (neighborhood symmetry of 2-order) | Information indices |  |
| 271 | IC3 | Information Content index (neighborhood symmetry of 3-order) | Information indices |  |
| 272 | TIC3 | Total Information Content index (neighborhood symmetry of 3-order) | Information indices |  |
| 273 | SIC3 | Structural Information Content index (neighborhood symmetry of 3-order) | Information indices |  |
| 274 | CIC3 | Complementary Information Content index (neighborhood symmetry of 3-order) | Information indices |  |
| 275 | BIC3 | Bond Information Content index (neighborhood symmetry of 3-order) | Information indices |  |
| 276 | IC4 | Information Content index (neighborhood symmetry of 4-order) | Information indices |  |
| 277 | TIC4 | Total Information Content index (neighborhood symmetry of 4-order) | Information indices |  |
| 278 | SIC4 | Structural Information Content index (neighborhood symmetry of 4-order) | Information indices |  |
| 279 | CIC4 | Complementary Information Content index (neighborhood symmetry of 4-order) | Information indices |  |
| 280 | BIC4 | Bond Information Content index (neighborhood symmetry of 4-order) | Information indices |  |
| 281 | IC5 | Information Content index (neighborhood symmetry of 5-order) | Information indices |  |
| 282 | TIC5 | Total Information Content index (neighborhood symmetry of 5-order) | Information indices |  |
| 283 | SIC5 | Structural Information Content index (neighborhood symmetry of 5-order) | Information indices |  |
| 284 | CIC5 | Complementary Information Content index (neighborhood symmetry of 5-order) | Information indices |  |
| 285 | BIC5 | Bond Information Content index (neighborhood symmetry of 5-order) | Information indices |  |
| 286 | ATS1m | Broto-Moreau autocorrelation of lag 1 (log function) weighted by mass | 2D autocorrelations |  |
| 287 | ATS2m | Broto-Moreau autocorrelation of lag 2 (log function) weighted by mass | 2D autocorrelations |  |
| 288 | ATS3m | Broto-Moreau autocorrelation of lag 3 (log function) weighted by mass | 2D autocorrelations |  |
| 289 | ATS4m | Broto-Moreau autocorrelation of lag 4 (log function) weighted by mass | 2D autocorrelations |  |
| 290 | ATS5m | Broto-Moreau autocorrelation of lag 5 (log function) weighted by mass | 2D autocorrelations |  |
| 291 | ATS6m | Broto-Moreau autocorrelation of lag 6 (log function) weighted by mass | 2D autocorrelations |  |
| 292 | ATS7m | Broto-Moreau autocorrelation of lag 7 (log function) weighted by mass | 2D autocorrelations |  |
| 293 | ATS8m | Broto-Moreau autocorrelation of lag 8 (log function) weighted by mass | 2D autocorrelations |  |
| 294 | ATS1v | Broto-Moreau autocorrelation of lag 1 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 295 | ATS2v | Broto-Moreau autocorrelation of lag 2 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 296 | ATS3v | Broto-Moreau autocorrelation of lag 3 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 297 | ATS4v | Broto-Moreau autocorrelation of lag 4 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 298 | ATS5v | Broto-Moreau autocorrelation of lag 5 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 299 | ATS6v | Broto-Moreau autocorrelation of lag 6 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 300 | ATS7v | Broto-Moreau autocorrelation of lag 7 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 301 | ATS8v | Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume | 2D autocorrelations |  |
| 302 | ATS1e | Broto-Moreau autocorrelation of lag 1 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 303 | ATS2e | Broto-Moreau autocorrelation of lag 2 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 304 | ATS3e | Broto-Moreau autocorrelation of lag 3 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 305 | ATS4e | Broto-Moreau autocorrelation of lag 4 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 306 | ATS5e | Broto-Moreau autocorrelation of lag 5 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 307 | ATS6e | Broto-Moreau autocorrelation of lag 6 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 308 | ATS7e | Broto-Moreau autocorrelation of lag 7 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 309 | ATS8e | Broto-Moreau autocorrelation of lag 8 (log function) weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 310 | ATS1p | Broto-Moreau autocorrelation of lag 1 (log function) weighted by polarizability | 2D autocorrelations |  |
| 311 | ATS2p | Broto-Moreau autocorrelation of lag 2 (log function) weighted by polarizability | 2D autocorrelations |  |
| 312 | ATS3p | Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability | 2D autocorrelations |  |
| 313 | ATS4p | Broto-Moreau autocorrelation of lag 4 (log function) weighted by polarizability | 2D autocorrelations |  |
| 314 | ATS5p | Broto-Moreau autocorrelation of lag 5 (log function) weighted by polarizability | 2D autocorrelations |  |
| 315 | ATS6p | Broto-Moreau autocorrelation of lag 6 (log function) weighted by polarizability | 2D autocorrelations |  |
| 316 | ATS7p | Broto-Moreau autocorrelation of lag 7 (log function) weighted by polarizability | 2D autocorrelations |  |
| 317 | ATS8p | Broto-Moreau autocorrelation of lag 8 (log function) weighted by polarizability | 2D autocorrelations |  |
| 318 | MATS1m | Moran autocorrelation of lag 1 weighted by mass | 2D autocorrelations |  |
| 319 | MATS2m | Moran autocorrelation of lag 2 weighted by mass | 2D autocorrelations |  |
| 320 | MATS3m | Moran autocorrelation of lag 3 weighted by mass | 2D autocorrelations |  |
| 321 | MATS4m | Moran autocorrelation of lag 4 weighted by mass | 2D autocorrelations |  |
| 322 | MATS5m | Moran autocorrelation of lag 5 weighted by mass | 2D autocorrelations |  |
| 323 | MATS6m | Moran autocorrelation of lag 6 weighted by mass | 2D autocorrelations |  |
| 324 | MATS7m | Moran autocorrelation of lag 7 weighted by mass | 2D autocorrelations |  |
| 325 | MATS8m | Moran autocorrelation of lag 8 weighted by mass | 2D autocorrelations |  |
| 326 | MATS1v | Moran autocorrelation of lag 1 weighted by van der Waals volume | 2D autocorrelations |  |
| 327 | MATS2v | Moran autocorrelation of lag 2 weighted by van der Waals volume | 2D autocorrelations |  |
| 328 | MATS3v | Moran autocorrelation of lag 3 weighted by van der Waals volume | 2D autocorrelations |  |
| 329 | MATS4v | Moran autocorrelation of lag 4 weighted by van der Waals volume | 2D autocorrelations |  |
| 330 | MATS5v | Moran autocorrelation of lag 5 weighted by van der Waals volume | 2D autocorrelations |  |
| 331 | MATS6v | Moran autocorrelation of lag 6 weighted by van der Waals volume | 2D autocorrelations |  |
| 332 | MATS7v | Moran autocorrelation of lag 7 weighted by van der Waals volume | 2D autocorrelations |  |
| 333 | MATS8v | Moran autocorrelation of lag 8 weighted by van der Waals volume | 2D autocorrelations |  |
| 334 | MATS1e | Moran autocorrelation of lag 1 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 335 | MATS2e | Moran autocorrelation of lag 2 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 336 | MATS3e | Moran autocorrelation of lag 3 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 337 | MATS4e | Moran autocorrelation of lag 4 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 338 | MATS5e | Moran autocorrelation of lag 5 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 339 | MATS6e | Moran autocorrelation of lag 6 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 340 | MATS7e | Moran autocorrelation of lag 7 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 341 | MATS8e | Moran autocorrelation of lag 8 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 342 | MATS1p | Moran autocorrelation of lag 1 weighted by polarizability | 2D autocorrelations |  |
| 343 | MATS2p | Moran autocorrelation of lag 2 weighted by polarizability | 2D autocorrelations |  |
| 344 | MATS3p | Moran autocorrelation of lag 3 weighted by polarizability | 2D autocorrelations |  |
| 345 | MATS4p | Moran autocorrelation of lag 4 weighted by polarizability | 2D autocorrelations |  |
| 346 | MATS5p | Moran autocorrelation of lag 5 weighted by polarizability | 2D autocorrelations |  |
| 347 | MATS6p | Moran autocorrelation of lag 6 weighted by polarizability | 2D autocorrelations |  |
| 348 | MATS7p | Moran autocorrelation of lag 7 weighted by polarizability | 2D autocorrelations |  |
| 349 | MATS8p | Moran autocorrelation of lag 8 weighted by polarizability | 2D autocorrelations |  |
| 350 | GATS1m | Geary autocorrelation of lag 1 weighted by mass | 2D autocorrelations |  |
| 351 | GATS2m | Geary autocorrelation of lag 2 weighted by mass | 2D autocorrelations |  |
| 352 | GATS3m | Geary autocorrelation of lag 3 weighted by mass | 2D autocorrelations |  |
| 353 | GATS4m | Geary autocorrelation of lag 4 weighted by mass | 2D autocorrelations |  |
| 354 | GATS5m | Geary autocorrelation of lag 5 weighted by mass | 2D autocorrelations |  |
| 355 | GATS6m | Geary autocorrelation of lag 6 weighted by mass | 2D autocorrelations |  |
| 356 | GATS7m | Geary autocorrelation of lag 7 weighted by mass | 2D autocorrelations |  |
| 357 | GATS8m | Geary autocorrelation of lag 8 weighted by mass | 2D autocorrelations |  |
| 358 | GATS1v | Geary autocorrelation of lag 1 weighted by van der Waals volume | 2D autocorrelations |  |
| 359 | GATS2v | Geary autocorrelation of lag 2 weighted by van der Waals volume | 2D autocorrelations |  |
| 360 | GATS3v | Geary autocorrelation of lag 3 weighted by van der Waals volume | 2D autocorrelations |  |
| 361 | GATS4v | Geary autocorrelation of lag 4 weighted by van der Waals volume | 2D autocorrelations |  |
| 362 | GATS5v | Geary autocorrelation of lag 5 weighted by van der Waals volume | 2D autocorrelations |  |
| 363 | GATS6v | Geary autocorrelation of lag 6 weighted by van der Waals volume | 2D autocorrelations |  |
| 364 | GATS7v | Geary autocorrelation of lag 7 weighted by van der Waals volume | 2D autocorrelations |  |
| 365 | GATS8v | Geary autocorrelation of lag 8 weighted by van der Waals volume | 2D autocorrelations |  |
| 366 | GATS1e | Geary autocorrelation of lag 1 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 367 | GATS2e | Geary autocorrelation of lag 2 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 368 | GATS3e | Geary autocorrelation of lag 3 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 369 | GATS4e | Geary autocorrelation of lag 4 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 370 | GATS5e | Geary autocorrelation of lag 5 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 371 | GATS6e | Geary autocorrelation of lag 6 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 372 | GATS7e | Geary autocorrelation of lag 7 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 373 | GATS8e | Geary autocorrelation of lag 8 weighted by Sanderson electronegativity | 2D autocorrelations |  |
| 374 | GATS1p | Geary autocorrelation of lag 1 weighted by polarizability | 2D autocorrelations |  |
| 375 | GATS2p | Geary autocorrelation of lag 2 weighted by polarizability | 2D autocorrelations |  |
| 376 | GATS3p | Geary autocorrelation of lag 3 weighted by polarizability | 2D autocorrelations |  |
| 377 | GATS4p | Geary autocorrelation of lag 4 weighted by polarizability | 2D autocorrelations |  |
| 378 | GATS5p | Geary autocorrelation of lag 5 weighted by polarizability | 2D autocorrelations |  |
| 379 | GATS6p | Geary autocorrelation of lag 6 weighted by polarizability | 2D autocorrelations |  |
| 380 | GATS7p | Geary autocorrelation of lag 7 weighted by polarizability | 2D autocorrelations |  |
| 381 | GATS8p | Geary autocorrelation of lag 8 weighted by polarizability | 2D autocorrelations |  |
| 382 | Chi0\_EA | Edge adjacency indices | Connectivity-like indices |  |
| 383 | Chi1\_EA | Edge adjacency indices | Connectivity-like indices |  |
| 384 | Eig01\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 385 | Eig02\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 386 | Eig03\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 387 | Eig04\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 388 | Eig05\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 389 | Eig06\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 390 | Eig07\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 391 | Eig08\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 392 | Eig09\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 393 | Eig10\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 394 | Eig11\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 395 | Eig12\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 396 | Eig13\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 397 | Eig14\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 398 | Eig15\_AEA(bo) | Edge adjacency indices | Eigenvalues |  |
| 399 | Eig01\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 400 | Eig02\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 401 | Eig03\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 402 | Eig04\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 403 | Eig05\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 404 | Eig06\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 405 | Eig07\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 406 | Eig08\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 407 | Eig09\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 408 | Eig10\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 409 | Eig11\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 410 | Eig12\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 411 | Eig13\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 412 | Eig14\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 413 | Eig15\_AEA(dm) | Edge adjacency indices | Eigenvalues |  |
| 414 | Eig01\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 415 | Eig02\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 416 | Eig03\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 417 | Eig04\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 418 | Eig05\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 419 | Eig06\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 420 | Eig07\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 421 | Eig08\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 422 | Eig09\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 423 | Eig10\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 424 | Eig11\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 425 | Eig12\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 426 | Eig13\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 427 | Eig14\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 428 | Eig15\_AEA(ri) | Edge adjacency indices | Eigenvalues |  |
| 429 | SM02\_EA | Edge adjacency indices | Spectral moments |  |
| 430 | SM03\_EA | Edge adjacency indices | Spectral moments |  |
| 431 | SM04\_EA | Edge adjacency indices | Spectral moments |  |
| 432 | SM05\_EA | Edge adjacency indices | Spectral moments |  |
| 433 | SM06\_EA | Edge adjacency indices | Spectral moments |  |
| 434 | SM07\_EA | Edge adjacency indices | Spectral moments |  |
| 435 | SM08\_EA | Edge adjacency indices | Spectral moments |  |
| 436 | SM09\_EA | Edge adjacency indices | Spectral moments |  |
| 437 | SM10\_EA | Edge adjacency indices | Spectral moments |  |
| 438 | SM11\_EA | Edge adjacency indices | Spectral moments |  |
| 439 | SM12\_EA | Edge adjacency indices | Spectral moments |  |
| 440 | SM13\_EA | Edge adjacency indices | Spectral moments |  |
| 441 | SM14\_EA | Edge adjacency indices | Spectral moments |  |
| 442 | SM15\_EA | Edge adjacency indices | Spectral moments |  |
| 443 | SM01\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 444 | SM02\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 445 | SM03\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 446 | SM04\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 447 | SM05\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 448 | SM06\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 449 | SM07\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 450 | SM08\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 451 | SM09\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 452 | SM10\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 453 | SM11\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 454 | SM12\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 455 | SM13\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 456 | SM14\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 457 | SM15\_AEA(bo) | Edge adjacency indices | Spectral moments |  |
| 458 | SM01\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 459 | SM02\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 460 | SM03\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 461 | SM04\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 462 | SM05\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 463 | SM06\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 464 | SM07\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 465 | SM08\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 466 | SM09\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 467 | SM10\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 468 | SM11\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 469 | SM12\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 470 | SM13\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 471 | SM14\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 472 | SM15\_AEA(dm) | Edge adjacency indices | Spectral moments |  |
| 473 | SM01\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 474 | SM02\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 475 | SM03\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 476 | SM04\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 477 | SM05\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 478 | SM06\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 479 | SM07\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 480 | SM08\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 481 | SM09\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 482 | SM10\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 483 | SM11\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 484 | SM12\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 485 | SM13\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 486 | SM14\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 487 | SM15\_AEA(ri) | Edge adjacency indices | Spectral moments |  |
| 488 | SpMax1\_Bh(m) | largest eigenvalue n. 1 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 489 | SpMax2\_Bh(m) | largest eigenvalue n. 2 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 490 | SpMax3\_Bh(m) | largest eigenvalue n. 3 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 491 | SpMax4\_Bh(m) | largest eigenvalue n. 4 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 492 | SpMax5\_Bh(m) | largest eigenvalue n. 5 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 493 | SpMax6\_Bh(m) | largest eigenvalue n. 6 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 494 | SpMax7\_Bh(m) | largest eigenvalue n. 7 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 495 | SpMax8\_Bh(m) | largest eigenvalue n. 8 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 496 | SpMin1\_Bh(m) | smallest eigenvalue n. 1 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 497 | SpMin2\_Bh(m) | smallest eigenvalue n. 2 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 498 | SpMin3\_Bh(m) | smallest eigenvalue n. 3 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 499 | SpMin4\_Bh(m) | smallest eigenvalue n. 4 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 500 | SpMin5\_Bh(m) | smallest eigenvalue n. 5 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 501 | SpMin6\_Bh(m) | smallest eigenvalue n. 6 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 502 | SpMin7\_Bh(m) | smallest eigenvalue n. 7 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 503 | SpMin8\_Bh(m) | smallest eigenvalue n. 8 of Burden matrix weighted by mass | Burden eigenvalues |  |
| 504 | SpMax1\_Bh(v) | largest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 505 | SpMax2\_Bh(v) | largest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 506 | SpMax3\_Bh(v) | largest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 507 | SpMax4\_Bh(v) | largest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 508 | SpMax5\_Bh(v) | largest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 509 | SpMax6\_Bh(v) | largest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 510 | SpMax7\_Bh(v) | largest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 511 | SpMax8\_Bh(v) | largest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 512 | SpMin1\_Bh(v) | smallest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 513 | SpMin2\_Bh(v) | smallest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 514 | SpMin3\_Bh(v) | smallest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 515 | SpMin4\_Bh(v) | smallest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 516 | SpMin5\_Bh(v) | smallest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 517 | SpMin6\_Bh(v) | smallest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 518 | SpMin7\_Bh(v) | smallest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 519 | SpMin8\_Bh(v) | smallest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume | Burden eigenvalues |  |
| 520 | SpMax1\_Bh(e) | largest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 521 | SpMax2\_Bh(e) | largest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 522 | SpMax3\_Bh(e) | largest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 523 | SpMax4\_Bh(e) | largest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 524 | SpMax5\_Bh(e) | largest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 525 | SpMax6\_Bh(e) | largest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 526 | SpMax7\_Bh(e) | largest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 527 | SpMax8\_Bh(e) | largest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 528 | SpMin1\_Bh(e) | smallest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 529 | SpMin2\_Bh(e) | smallest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 530 | SpMin3\_Bh(e) | smallest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 531 | SpMin4\_Bh(e) | smallest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 532 | SpMin5\_Bh(e) | smallest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 533 | SpMin6\_Bh(e) | smallest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 534 | SpMin7\_Bh(e) | smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 535 | SpMin8\_Bh(e) | smallest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity | Burden eigenvalues |  |
| 536 | SpMax1\_Bh(p) | largest eigenvalue n. 1 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 537 | SpMax2\_Bh(p) | largest eigenvalue n. 2 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 538 | SpMax3\_Bh(p) | largest eigenvalue n. 3 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 539 | SpMax4\_Bh(p) | largest eigenvalue n. 4 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 540 | SpMax5\_Bh(p) | largest eigenvalue n. 5 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 541 | SpMax6\_Bh(p) | largest eigenvalue n. 6 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 542 | SpMax7\_Bh(p) | largest eigenvalue n. 7 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 543 | SpMax8\_Bh(p) | largest eigenvalue n. 8 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 544 | SpMin1\_Bh(p) | smallest eigenvalue n. 1 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 545 | SpMin2\_Bh(p) | smallest eigenvalue n. 2 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 546 | SpMin3\_Bh(p) | smallest eigenvalue n. 3 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 547 | SpMin4\_Bh(p) | smallest eigenvalue n. 4 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 548 | SpMin5\_Bh(p) | smallest eigenvalue n. 5 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 549 | SpMin6\_Bh(p) | smallest eigenvalue n. 6 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 550 | SpMin7\_Bh(p) | smallest eigenvalue n. 7 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 551 | SpMin8\_Bh(p) | smallest eigenvalue n. 8 of Burden matrix weighted by polarizability | Burden eigenvalues |  |
| 552 | GGI1 | topological charge index of order 1 | 2D autocorrelations |  |
| 553 | GGI2 | topological charge index of order 2 | 2D autocorrelations |  |
| 554 | GGI3 | topological charge index of order 3 | 2D autocorrelations |  |
| 555 | GGI4 | topological charge index of order 4 | 2D autocorrelations |  |
| 556 | GGI5 | topological charge index of order 5 | 2D autocorrelations |  |
| 557 | GGI6 | topological charge index of order 6 | 2D autocorrelations |  |
| 558 | GGI7 | topological charge index of order 7 | 2D autocorrelations |  |
| 559 | GGI8 | topological charge index of order 8 | 2D autocorrelations |  |
| 560 | GGI9 | topological charge index of order 9 | 2D autocorrelations |  |
| 561 | GGI10 | topological charge index of order 10 | 2D autocorrelations |  |
| 562 | JGI1 | mean topological charge index of order 1 | 2D autocorrelations |  |
| 563 | JGI2 | mean topological charge index of order 2 | 2D autocorrelations |  |
| 564 | JGI3 | mean topological charge index of order 3 | 2D autocorrelations |  |
| 565 | JGI4 | mean topological charge index of order 4 | 2D autocorrelations |  |
| 566 | JGI5 | mean topological charge index of order 5 | 2D autocorrelations |  |
| 567 | JGI6 | mean topological charge index of order 6 | 2D autocorrelations |  |
| 568 | JGI7 | mean topological charge index of order 7 | 2D autocorrelations |  |
| 569 | JGI8 | mean topological charge index of order 8 | 2D autocorrelations |  |
| 570 | JGI9 | mean topological charge index of order 9 | 2D autocorrelations |  |
| 571 | JGI10 | mean topological charge index of order 10 | 2D autocorrelations |  |
| 572 | JGT | global topological charge index | 2D autocorrelations |  |
| 573 | SpMax\_A | Adjacency matrix (A) | 2D matrix-based descriptors |  |
| 574 | SpMax\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 575 | SpMax\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 576 | SpMax\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 577 | SpMax\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 578 | SpMax\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 579 | SM1\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 580 | SM1\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 581 | SM1\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 582 | SM1\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 583 | SM1\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 584 | SpAbs\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 585 | SpAbs\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 586 | SpAbs\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 587 | SpAbs\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 588 | SpAbs\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 589 | VE1\_A | Adjacency matrix (A) | 2D matrix-based descriptors |  |
| 590 | VE2\_A | Adjacency matrix (A) | 2D matrix-based descriptors |  |
| 591 | VR1\_A | Adjacency matrix (A) | 2D matrix-based descriptors |  |
| 592 | VR2\_A | Adjacency matrix (A) | 2D matrix-based descriptors |  |
| 593 | VE1\_D | Topological distance matrix (D) | 2D matrix-based descriptors |  |
| 594 | VE2\_D | Topological distance matrix (D) | 2D matrix-based descriptors |  |
| 595 | VR1\_D | Topological distance matrix (D) | 2D matrix-based descriptors |  |
| 596 | VR2\_D | Topological distance matrix (D) | 2D matrix-based descriptors |  |
| 597 | VE1\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 598 | VE2\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 599 | VR1\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 600 | VR2\_Dz(Z) | Barysz matrix weighted by atomic number (Dz(Z)) | 2D matrix-based descriptors |  |
| 601 | VE1\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 602 | VE2\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 603 | VR1\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 604 | VR2\_Dz(m) | Barysz matrix weighted by mass (Dz(m)) | 2D matrix-based descriptors |  |
| 605 | VE1\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 606 | VE2\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 607 | VR1\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 608 | VR2\_Dz(v) | Barysz matrix weighted by Van der Waals volume (Dz(v)) | 2D matrix-based descriptors |  |
| 609 | VE1\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 610 | VE2\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 611 | VR1\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 612 | VR2\_Dz(e) | Barysz matrix weighted by Sanderson electronegativity (Dz(e)) | 2D matrix-based descriptors |  |
| 613 | VE1\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 614 | VE2\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 615 | VR1\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 616 | VR2\_Dz(p) | Barysz matrix weighted by polarizability (Dz(p)) | 2D matrix-based descriptors |  |
| 617 | DP01 | molecular profile no. 1 | Randic molecular profiles |  |
| 618 | DP02 | molecular profile no. 2 | Randic molecular profiles |  |
| 619 | DP03 | molecular profile no. 3 | Randic molecular profiles |  |
| 620 | DP04 | molecular profile no. 4 | Randic molecular profiles |  |
| 621 | DP05 | molecular profile no. 5 | Randic molecular profiles |  |
| 622 | DP06 | molecular profile no. 6 | Randic molecular profiles |  |
| 623 | DP07 | molecular profile no. 7 | Randic molecular profiles |  |
| 624 | DP08 | molecular profile no. 8 | Randic molecular profiles |  |
| 625 | DP09 | molecular profile no. 9 | Randic molecular profiles |  |
| 626 | DP10 | molecular profile no. 10 | Randic molecular profiles |  |
| 627 | DP11 | molecular profile no. 11 | Randic molecular profiles |  |
| 628 | DP12 | molecular profile no. 12 | Randic molecular profiles |  |
| 629 | DP13 | molecular profile no. 13 | Randic molecular profiles |  |
| 630 | DP14 | molecular profile no. 14 | Randic molecular profiles |  |
| 631 | DP15 | molecular profile no. 15 | Randic molecular profiles |  |
| 632 | DP16 | molecular profile no. 16 | Randic molecular profiles |  |
| 633 | DP17 | molecular profile no. 17 | Randic molecular profiles |  |
| 634 | DP18 | molecular profile no. 18 | Randic molecular profiles |  |
| 635 | DP19 | molecular profile no. 19 | Randic molecular profiles |  |
| 636 | DP20 | molecular profile no. 20 | Randic molecular profiles |  |
| 637 | SP01 | shape profile no. 1 | Randic molecular profiles |  |
| 638 | SP02 | shape profile no. 2 | Randic molecular profiles |  |
| 639 | SP03 | shape profile no. 3 | Randic molecular profiles |  |
| 640 | SP04 | shape profile no. 4 | Randic molecular profiles |  |
| 641 | SP05 | shape profile no. 5 | Randic molecular profiles |  |
| 642 | SP06 | shape profile no. 6 | Randic molecular profiles |  |
| 643 | SP07 | shape profile no. 7 | Randic molecular profiles |  |
| 644 | SP08 | shape profile no. 8 | Randic molecular profiles |  |
| 645 | SP09 | shape profile no. 9 | Randic molecular profiles |  |
| 646 | SP10 | shape profile no. 10 | Randic molecular profiles |  |
| 647 | SP11 | shape profile no. 11 | Randic molecular profiles |  |
| 648 | SP12 | shape profile no. 12 | Randic molecular profiles |  |
| 649 | SP13 | shape profile no. 13 | Randic molecular profiles |  |
| 650 | SP14 | shape profile no. 14 | Randic molecular profiles |  |
| 651 | SP15 | shape profile no. 15 | Randic molecular profiles |  |
| 652 | SP16 | shape profile no. 16 | Randic molecular profiles |  |
| 653 | SP17 | shape profile no. 17 | Randic molecular profiles |  |
| 654 | SP18 | shape profile no. 18 | Randic molecular profiles |  |
| 655 | SP19 | shape profile no. 19 | Randic molecular profiles |  |
| 656 | SP20 | shape profile no. 20 | Randic molecular profiles |  |
| 657 | SHP2 | average shape profile index of order 2 | Randic molecular profiles |  |
| 658 | W3D | 3D-Wiener index | Geometrical descriptors |  |
| 659 | J3D | 3D-Balaban index | Geometrical descriptors |  |
| 660 | H3D | 3D-Harary index | Geometrical descriptors |  |
| 661 | AGDD | average geometric distance degree | Geometrical descriptors |  |
| 662 | DDI | D/D index | Geometrical descriptors |  |
| 663 | ADDD | average distance/distance degree | Geometrical descriptors |  |
| 664 | G1 | gravitational index G1 | Geometrical descriptors |  |
| 665 | G2 | gravitational index G2 (bond-restricted) | Geometrical descriptors |  |
| 666 | RGyr | radius of gyration (mass weighted) | Geometrical descriptors |  |
| 667 | SPAN | span R | Geometrical descriptors |  |
| 668 | SPAM | average span R | Geometrical descriptors |  |
| 669 | MEcc | molecular eccentricity | Geometrical descriptors |  |
| 670 | SPH | spherosity | Geometrical descriptors |  |
| 671 | ASP | asphericity | Geometrical descriptors |  |
| 672 | FDI | folding degree index | Geometrical descriptors |  |
| 673 | PJI3 | 3D Petitjean shape index | Geometrical descriptors |  |
| 674 | L/Bw | length-to-breadth ratio by WHIM | Geometrical descriptors |  |
| 675 | HOMA | Harmonic Oscillator Model of Aromaticity index | Geometrical descriptors |  |
| 676 | CMBL | conjugated maximum bond length | Geometrical descriptors |  |
| 677 | RCI | Jug RC index | Geometrical descriptors |  |
| 678 | AROM | aromaticity index | Geometrical descriptors |  |
| 679 | HOMT | HOMA total | Geometrical descriptors |  |
| 680 | DISPm | displacement value / weighted by mass | Geometrical descriptors |  |
| 681 | QXXm | quadrupole x-component value / weighted by mass | Geometrical descriptors |  |
| 682 | QYYm | quadrupole y-component value / weighted by mass | Geometrical descriptors |  |
| 683 | QZZm | quadrupole z-component value / weighted by mass | Geometrical descriptors |  |
| 684 | DISPv | displacement value / weighted by van der Waals volume | Geometrical descriptors |  |
| 685 | QXXv | quadrupole x-component value / weighted by van der Waals volume | Geometrical descriptors |  |
| 686 | QYYv | quadrupole y-component value / weighted by van der Waals volume | Geometrical descriptors |  |
| 687 | QZZv | quadrupole z-component value / weighted by van der Waals volume | Geometrical descriptors |  |
| 688 | DISPe | displacement value / weighted by Sanderson electronegativity | Geometrical descriptors |  |
| 689 | QXXe | quadrupole x-component value / weighted by Sanderson electronegativity | Geometrical descriptors |  |
| 690 | QYYe | quadrupole y-component value / weighted by Sanderson electronegativity | Geometrical descriptors |  |
| 691 | QZZe | quadrupole z-component value / weighted by Sanderson electronegativity | Geometrical descriptors |  |
| 692 | DISPp | displacement value / weighted by polarizability | Geometrical descriptors |  |
| 693 | QXXp | quadrupole x-component value / weighted by polarizability | Geometrical descriptors |  |
| 694 | QYYp | quadrupole y-component value / weighted by polarizability | Geometrical descriptors |  |
| 695 | QZZp | quadrupole z-component value / weighted by polarizability | Geometrical descriptors |  |
| 696 | G(N..N) | sum of geometrical distances between N..N | 3D Atom Pairs |  |
| 697 | G(N..O) | sum of geometrical distances between N..O | 3D Atom Pairs |  |
| 698 | G(N..S) | sum of geometrical distances between N..S | 3D Atom Pairs |  |
| 699 | G(N..P) | sum of geometrical distances between N..P | 3D Atom Pairs |  |
| 700 | G(N..F) | sum of geometrical distances between N..F | 3D Atom Pairs |  |
| 701 | G(N..Cl) | sum of geometrical distances between N..Cl | 3D Atom Pairs |  |
| 702 | G(N..Br) | sum of geometrical distances between N..Br | 3D Atom Pairs |  |
| 703 | G(N..I) | sum of geometrical distances between N..I | 3D Atom Pairs |  |
| 704 | G(O..O) | sum of geometrical distances between O..O | 3D Atom Pairs |  |
| 705 | G(O..S) | sum of geometrical distances between O..S | 3D Atom Pairs |  |
| 706 | G(O..P) | sum of geometrical distances between O..P | 3D Atom Pairs |  |
| 707 | G(O..F) | sum of geometrical distances between O..F | 3D Atom Pairs |  |
| 708 | G(O..Cl) | sum of geometrical distances between O..Cl | 3D Atom Pairs |  |
| 709 | G(O..Br) | sum of geometrical distances between O..Br | 3D Atom Pairs |  |
| 710 | G(O..I) | sum of geometrical distances between O..I | 3D Atom Pairs |  |
| 711 | G(S..S) | sum of geometrical distances between S..S | 3D Atom Pairs |  |
| 712 | G(S..P) | sum of geometrical distances between S..P | 3D Atom Pairs |  |
| 713 | G(S..F) | sum of geometrical distances between S..F | 3D Atom Pairs |  |
| 714 | G(S..Cl) | sum of geometrical distances between S..Cl | 3D Atom Pairs |  |
| 715 | G(S..Br) | sum of geometrical distances between S..Br | 3D Atom Pairs |  |
| 716 | G(S..I) | sum of geometrical distances between S..I | 3D Atom Pairs |  |
| 717 | G(P..P) | sum of geometrical distances between P..P | 3D Atom Pairs |  |
| 718 | G(P..F) | sum of geometrical distances between P..F | 3D Atom Pairs |  |
| 719 | G(P..Cl) | sum of geometrical distances between P..Cl | 3D Atom Pairs |  |
| 720 | G(P..Br) | sum of geometrical distances between P..Br | 3D Atom Pairs |  |
| 721 | G(P..I) | sum of geometrical distances between P..I | 3D Atom Pairs |  |
| 722 | G(F..F) | sum of geometrical distances between F..F | 3D Atom Pairs |  |
| 723 | G(F..Cl) | sum of geometrical distances between F..Cl | 3D Atom Pairs |  |
| 724 | G(Br..Br) | sum of geometrical distances between Br..Br | 3D Atom Pairs |  |
| 725 | RDF010u | Radial Distribution Function - 010 / unweighted RDF descriptors | RDF descriptors |  |
| 726 | RDF015u | Radial Distribution Function - 015 / unweighted RDF descriptors | RDF descriptors |  |
| 727 | RDF020u | Radial Distribution Function - 020 / unweighted RDF descriptors | RDF descriptors |  |
| 728 | RDF025u | Radial Distribution Function - 025 / unweighted RDF descriptors | RDF descriptors |  |
| 729 | RDF030u | Radial Distribution Function - 030 / unweighted RDF descriptors | RDF descriptors |  |
| 730 | RDF035u | Radial Distribution Function - 035 / unweighted RDF descriptors | RDF descriptors |  |
| 731 | RDF040u | Radial Distribution Function - 040 / unweighted RDF descriptors | RDF descriptors |  |
| 732 | RDF045u | Radial Distribution Function - 045 / unweighted RDF descriptors | RDF descriptors |  |
| 733 | RDF050u | Radial Distribution Function - 050 / unweighted RDF descriptors | RDF descriptors |  |
| 734 | RDF055u | Radial Distribution Function - 055 / unweighted RDF descriptors | RDF descriptors |  |
| 735 | RDF060u | Radial Distribution Function - 060 / unweighted RDF descriptors | RDF descriptors |  |
| 736 | RDF065u | Radial Distribution Function - 065 / unweighted RDF descriptors | RDF descriptors |  |
| 737 | RDF070u | Radial Distribution Function - 070 / unweighted RDF descriptors | RDF descriptors |  |
| 738 | RDF075u | Radial Distribution Function - 075 / unweighted RDF descriptors | RDF descriptors |  |
| 739 | RDF080u | Radial Distribution Function - 080 / unweighted RDF descriptors | RDF descriptors |  |
| 740 | RDF085u | Radial Distribution Function - 085 / unweighted RDF descriptors | RDF descriptors |  |
| 741 | RDF090u | Radial Distribution Function - 090 / unweighted RDF descriptors | RDF descriptors |  |
| 742 | RDF095u | Radial Distribution Function - 095 / unweighted RDF descriptors | RDF descriptors |  |
| 743 | RDF100u | Radial Distribution Function - 100 / unweighted RDF descriptors | RDF descriptors |  |
| 744 | RDF105u | Radial Distribution Function - 105 / unweighted RDF descriptors | RDF descriptors |  |
| 745 | RDF110u | Radial Distribution Function - 110 / unweighted RDF descriptors | RDF descriptors |  |
| 746 | RDF115u | Radial Distribution Function - 115 / unweighted RDF descriptors | RDF descriptors |  |
| 747 | RDF120u | Radial Distribution Function - 120 / unweighted RDF descriptors | RDF descriptors |  |
| 748 | RDF125u | Radial Distribution Function - 125 / unweighted RDF descriptors | RDF descriptors |  |
| 749 | RDF130u | Radial Distribution Function - 130 / unweighted RDF descriptors | RDF descriptors |  |
| 750 | RDF135u | Radial Distribution Function - 135 / unweighted RDF descriptors | RDF descriptors |  |
| 751 | RDF140u | Radial Distribution Function - 140 / unweighted RDF descriptors | RDF descriptors |  |
| 752 | RDF145u | Radial Distribution Function - 145 / unweighted RDF descriptors | RDF descriptors |  |
| 753 | RDF150u | Radial Distribution Function - 150 / unweighted RDF descriptors | RDF descriptors |  |
| 754 | RDF155u | Radial Distribution Function - 155 / unweighted RDF descriptors | RDF descriptors |  |
| 755 | RDF010m | Radial Distribution Function - 010 / weighted by mass | RDF descriptors |  |
| 756 | RDF015m | Radial Distribution Function - 015 / weighted by mass | RDF descriptors |  |
| 757 | RDF020m | Radial Distribution Function - 020 / weighted by mass | RDF descriptors |  |
| 758 | RDF025m | Radial Distribution Function - 025 / weighted by mass | RDF descriptors |  |
| 759 | RDF030m | Radial Distribution Function - 030 / weighted by mass | RDF descriptors |  |
| 760 | RDF035m | Radial Distribution Function - 035 / weighted by mass | RDF descriptors |  |
| 761 | RDF040m | Radial Distribution Function - 040 / weighted by mass | RDF descriptors |  |
| 762 | RDF045m | Radial Distribution Function - 045 / weighted by mass | RDF descriptors |  |
| 763 | RDF050m | Radial Distribution Function - 050 / weighted by mass | RDF descriptors |  |
| 764 | RDF055m | Radial Distribution Function - 055 / weighted by mass | RDF descriptors |  |
| 765 | RDF060m | Radial Distribution Function - 060 / weighted by mass | RDF descriptors |  |
| 766 | RDF065m | Radial Distribution Function - 065 / weighted by mass | RDF descriptors |  |
| 767 | RDF070m | Radial Distribution Function - 070 / weighted by mass | RDF descriptors |  |
| 768 | RDF075m | Radial Distribution Function - 075 / weighted by mass | RDF descriptors |  |
| 769 | RDF080m | Radial Distribution Function - 080 / weighted by mass | RDF descriptors |  |
| 770 | RDF085m | Radial Distribution Function - 085 / weighted by mass | RDF descriptors |  |
| 771 | RDF090m | Radial Distribution Function - 090 / weighted by mass | RDF descriptors |  |
| 772 | RDF095m | Radial Distribution Function - 095 / weighted by mass | RDF descriptors |  |
| 773 | RDF100m | Radial Distribution Function - 100 / weighted by mass | RDF descriptors |  |
| 774 | RDF105m | Radial Distribution Function - 105 / weighted by mass | RDF descriptors |  |
| 775 | RDF110m | Radial Distribution Function - 110 / weighted by mass | RDF descriptors |  |
| 776 | RDF115m | Radial Distribution Function - 115 / weighted by mass | RDF descriptors |  |
| 777 | RDF120m | Radial Distribution Function - 120 / weighted by mass | RDF descriptors |  |
| 778 | RDF125m | Radial Distribution Function - 125 / weighted by mass | RDF descriptors |  |
| 779 | RDF130m | Radial Distribution Function - 130 / weighted by mass | RDF descriptors |  |
| 780 | RDF135m | Radial Distribution Function - 135 / weighted by mass | RDF descriptors |  |
| 781 | RDF140m | Radial Distribution Function - 140 / weighted by mass | RDF descriptors |  |
| 782 | RDF145m | Radial Distribution Function - 145 / weighted by mass | RDF descriptors |  |
| 783 | RDF150m | Radial Distribution Function - 150 / weighted by mass | RDF descriptors |  |
| 784 | RDF155m | Radial Distribution Function - 155 / weighted by mass | RDF descriptors |  |
| 785 | RDF010v | Radial Distribution Function - 010 / weighted by van der Waals volum | RDF descriptors |  |
| 786 | RDF015v | Radial Distribution Function - 015 / weighted by van der Waals volum | RDF descriptors |  |
| 787 | RDF020v | Radial Distribution Function - 020 / weighted by van der Waals volum | RDF descriptors |  |
| 788 | RDF025v | Radial Distribution Function - 025 / weighted by van der Waals volum | RDF descriptors |  |
| 789 | RDF030v | Radial Distribution Function - 030 / weighted by van der Waals volum | RDF descriptors |  |
| 790 | RDF035v | Radial Distribution Function - 035/ weighted by van der Waals volum | RDF descriptors |  |
| 791 | RDF040v | Radial Distribution Function - 040/ weighted by van der Waals volum | RDF descriptors |  |
| 792 | RDF045v | Radial Distribution Function - 045 / weighted by van der Waals volum | RDF descriptors |  |
| 793 | RDF050v | Radial Distribution Function - 050 / weighted by van der Waals volum | RDF descriptors |  |
| 794 | RDF055v | Radial Distribution Function - 055 / weighted by van der Waals volum | RDF descriptors |  |
| 795 | RDF060v | Radial Distribution Function - 060 / weighted by van der Waals volum | RDF descriptors |  |
| 796 | RDF065v | Radial Distribution Function - 065 / weighted by van der Waals volum | RDF descriptors |  |
| 797 | RDF070v | Radial Distribution Function - 070/ weighted by van der Waals volum | RDF descriptors |  |
| 798 | RDF075v | Radial Distribution Function - 075 / weighted by van der Waals volum | RDF descriptors |  |
| 799 | RDF080v | Radial Distribution Function - 080 / weighted by van der Waals volum | RDF descriptors |  |
| 800 | RDF085v | Radial Distribution Function - 085 / weighted by van der Waals volum | RDF descriptors |  |
| 801 | RDF090v | Radial Distribution Function - 090 / weighted by van der Waals volum | RDF descriptors |  |
| 802 | RDF095v | Radial Distribution Function - 095 / weighted by van der Waals volum | RDF descriptors |  |
| 803 | RDF100v | Radial Distribution Function - 100 / weighted by van der Waals volum | RDF descriptors |  |
| 804 | RDF105v | Radial Distribution Function - 105 / weighted by van der Waals volum | RDF descriptors |  |
| 805 | RDF110v | Radial Distribution Function - 110 / weighted by van der Waals volum | RDF descriptors |  |
| 806 | RDF115v | Radial Distribution Function - 115 / weighted by van der Waals volum | RDF descriptors |  |
| 807 | RDF120v | Radial Distribution Function - 120 / weighted by van der Waals volum | RDF descriptors |  |
| 808 | RDF125v | Radial Distribution Function - 125/ weighted by van der Waals volum | RDF descriptors |  |
| 809 | RDF130v | Radial Distribution Function - 130 / weighted by van der Waals volum | RDF descriptors |  |
| 810 | RDF135v | Radial Distribution Function - 135 / weighted by van der Waals volum | RDF descriptors |  |
| 811 | RDF140v | Radial Distribution Function - 140 / weighted by van der Waals volum | RDF descriptors |  |
| 812 | RDF145v | Radial Distribution Function - 145 / weighted by van der Waals volum | RDF descriptors |  |
| 813 | RDF150v | Radial Distribution Function - 150 / weighted by van der Waals volum | RDF descriptors |  |
| 814 | RDF155v | Radial Distribution Function - 155 / weighted by van der Waals volum | RDF descriptors |  |
| 815 | RDF010e | Radial Distribution Function - 010 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 816 | RDF015e | Radial Distribution Function - 015 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 817 | RDF020e | Radial Distribution Function - 020 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 818 | RDF025e | Radial Distribution Function - 025 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 819 | RDF030e | Radial Distribution Function - 030 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 820 | RDF035e | Radial Distribution Function - 035 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 821 | RDF040e | Radial Distribution Function - 040 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 822 | RDF045e | Radial Distribution Function - 045 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 823 | RDF050e | Radial Distribution Function - 050 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 824 | RDF055e | Radial Distribution Function - 055 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 825 | RDF060e | Radial Distribution Function - 060 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 826 | RDF065e | Radial Distribution Function - 065 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 827 | RDF070e | Radial Distribution Function - 070 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 828 | RDF075e | Radial Distribution Function - 075 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 829 | RDF080e | Radial Distribution Function - 080 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 830 | RDF085e | Radial Distribution Function - 085 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 831 | RDF090e | Radial Distribution Function - 090 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 832 | RDF095e | Radial Distribution Function - 095 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 833 | RDF100e | Radial Distribution Function - 100 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 834 | RDF105e | Radial Distribution Function - 105 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 835 | RDF110e | Radial Distribution Function - 110 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 836 | RDF115e | Radial Distribution Function - 115 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 837 | RDF120e | Radial Distribution Function - 120 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 838 | RDF125e | Radial Distribution Function - 125 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 839 | RDF130e | Radial Distribution Function - 130 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 840 | RDF135e | Radial Distribution Function - 135/ weighted by Sanderson electronegativity | RDF descriptors |  |
| 841 | RDF140e | Radial Distribution Function - 140 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 842 | RDF145e | Radial Distribution Function - 145 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 843 | RDF150e | Radial Distribution Function - 150 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 844 | RDF155e | Radial Distribution Function - 155 / weighted by Sanderson electronegativity | RDF descriptors |  |
| 845 | RDF010p | Radial Distribution Function - 010 / weighted by polarizability | RDF descriptors |  |
| 846 | RDF015p | Radial Distribution Function - 015 / weighted by polarizability | RDF descriptors |  |
| 847 | RDF020p | Radial Distribution Function - 020 / weighted by polarizability | RDF descriptors |  |
| 848 | RDF025p | Radial Distribution Function - 025 / weighted by polarizability | RDF descriptors |  |
| 849 | RDF030p | Radial Distribution Function - 030 / weighted by polarizability | RDF descriptors |  |
| 850 | RDF035p | Radial Distribution Function - 035 / weighted by polarizability | RDF descriptors |  |
| 851 | RDF040p | Radial Distribution Function - 040 / weighted by polarizability | RDF descriptors |  |
| 852 | RDF045p | Radial Distribution Function - 045 / weighted by polarizability | RDF descriptors |  |
| 853 | RDF050p | Radial Distribution Function - 050 / weighted by polarizability | RDF descriptors |  |
| 854 | RDF055p | Radial Distribution Function - 055 / weighted by polarizability | RDF descriptors |  |
| 855 | RDF060p | Radial Distribution Function - 060 / weighted by polarizability | RDF descriptors |  |
| 856 | RDF065p | Radial Distribution Function - 065 / weighted by polarizability | RDF descriptors |  |
| 857 | RDF070p | Radial Distribution Function - 070 / weighted by polarizability | RDF descriptors |  |
| 858 | RDF075p | Radial Distribution Function - 075 / weighted by polarizability | RDF descriptors |  |
| 859 | RDF080p | Radial Distribution Function - 080 / weighted by polarizability | RDF descriptors |  |
| 860 | RDF085p | Radial Distribution Function - 085 / weighted by polarizability | RDF descriptors |  |
| 861 | RDF090p | Radial Distribution Function - 090 / weighted by polarizability | RDF descriptors |  |
| 862 | RDF095p | Radial Distribution Function - 095 / weighted by polarizability | RDF descriptors |  |
| 863 | RDF100p | Radial Distribution Function - 100 / weighted by polarizability | RDF descriptors |  |
| 864 | RDF105p | Radial Distribution Function - 105 / weighted by polarizability | RDF descriptors |  |
| 865 | RDF110p | Radial Distribution Function - 110 / weighted by polarizability | RDF descriptors |  |
| 866 | RDF115p | Radial Distribution Function - 115 / weighted by polarizability | RDF descriptors |  |
| 867 | RDF120p | Radial Distribution Function - 120 / weighted by polarizability | RDF descriptors |  |
| 868 | RDF125p | Radial Distribution Function - 125 / weighted by polarizability | RDF descriptors |  |
| 869 | RDF130p | Radial Distribution Function - 130 / weighted by polarizability | RDF descriptors |  |
| 870 | RDF135p | Radial Distribution Function - 135 / weighted by polarizability | RDF descriptors |  |
| 871 | RDF140p | Radial Distribution Function - 140 / weighted by polarizability | RDF descriptors |  |
| 872 | RDF145p | Radial Distribution Function - 145 / weighted by polarizability | RDF descriptors |  |
| 873 | RDF150p | Radial Distribution Function - 150 / weighted by polarizability | RDF descriptors |  |
| 874 | RDF155p | Radial Distribution Function - 155 / weighted by polarizability | RDF descriptors |  |
| 875 | Mor01u | signal 01 / unweighted | 3D-MoRSE descriptors |  |
| 876 | Mor02u | signal 02 / unweighted | 3D-MoRSE descriptors |  |
| 877 | Mor03u | signal 03 / unweighted | 3D-MoRSE descriptors |  |
| 878 | Mor04u | signal 04 / unweighted | 3D-MoRSE descriptors |  |
| 879 | Mor05u | signal 05 / unweighted | 3D-MoRSE descriptors |  |
| 880 | Mor06u | signal 06 / unweighted | 3D-MoRSE descriptors |  |
| 881 | Mor07u | signal 07 / unweighted | 3D-MoRSE descriptors |  |
| 882 | Mor08u | signal 08 / unweighted | 3D-MoRSE descriptors |  |
| 883 | Mor09u | signal 09 / unweighted | 3D-MoRSE descriptors |  |
| 884 | Mor10u | signal 10 / unweighted | 3D-MoRSE descriptors |  |
| 885 | Mor11u | signal 11 / unweighted | 3D-MoRSE descriptors |  |
| 886 | Mor12u | signal 12 / unweighted | 3D-MoRSE descriptors |  |
| 887 | Mor13u | signal 13 / unweighted | 3D-MoRSE descriptors |  |
| 888 | Mor14u | signal 14 / unweighted | 3D-MoRSE descriptors |  |
| 889 | Mor15u | signal 15 / unweighted | 3D-MoRSE descriptors |  |
| 890 | Mor16u | signal 16 / unweighted | 3D-MoRSE descriptors |  |
| 891 | Mor17u | signal 17 / unweighted | 3D-MoRSE descriptors |  |
| 892 | Mor18u | signal 18 / unweighted | 3D-MoRSE descriptors |  |
| 893 | Mor19u | signal 19 / unweighted | 3D-MoRSE descriptors |  |
| 894 | Mor20u | signal 20 / unweighted | 3D-MoRSE descriptors |  |
| 895 | Mor21u | signal 21 / unweighted | 3D-MoRSE descriptors |  |
| 896 | Mor22u | signal 22 / unweighted | 3D-MoRSE descriptors |  |
| 897 | Mor23u | signal 23 / unweighted | 3D-MoRSE descriptors |  |
| 898 | Mor24u | signal 24 / unweighted | 3D-MoRSE descriptors |  |
| 899 | Mor25u | signal 25 / unweighted | 3D-MoRSE descriptors |  |
| 900 | Mor26u | signal 26 / unweighted | 3D-MoRSE descriptors |  |
| 901 | Mor27u | signal 27 / unweighted | 3D-MoRSE descriptors |  |
| 902 | Mor28u | signal 28 / unweighted | 3D-MoRSE descriptors |  |
| 903 | Mor29u | signal 29 / unweighted | 3D-MoRSE descriptors |  |
| 904 | Mor30u | signal 30 / unweighted | 3D-MoRSE descriptors |  |
| 905 | Mor31u | signal 31 / unweighted | 3D-MoRSE descriptors |  |
| 906 | Mor32u | signal 32 / unweighted | 3D-MoRSE descriptors |  |
| 907 | Mor01m | signal 01 / weighted by mass | 3D-MoRSE descriptors |  |
| 908 | Mor02m | signal 02 / weighted by mass | 3D-MoRSE descriptors |  |
| 909 | Mor03m | signal 03 / weighted by mass | 3D-MoRSE descriptors |  |
| 910 | Mor04m | signal 04 / weighted by mass | 3D-MoRSE descriptors |  |
| 911 | Mor05m | signal 05 / weighted by mass | 3D-MoRSE descriptors |  |
| 912 | Mor06m | signal 06 / weighted by mass | 3D-MoRSE descriptors |  |
| 913 | Mor07m | signal 07 / weighted by mass | 3D-MoRSE descriptors |  |
| 914 | Mor08m | signal 08 / weighted by mass | 3D-MoRSE descriptors |  |
| 915 | Mor09m | signal 09 / weighted by mass | 3D-MoRSE descriptors |  |
| 916 | Mor10m | signal 10 / weighted by mass | 3D-MoRSE descriptors |  |
| 917 | Mor11m | signal 11 / weighted by mass | 3D-MoRSE descriptors |  |
| 918 | Mor12m | signal 12 / weighted by mass | 3D-MoRSE descriptors |  |
| 919 | Mor13m | signal 13 / weighted by mass | 3D-MoRSE descriptors |  |
| 920 | Mor14m | signal 14 / weighted by mass | 3D-MoRSE descriptors |  |
| 921 | Mor15m | signal 15 / weighted by mass | 3D-MoRSE descriptors |  |
| 922 | Mor16m | signal 16 / weighted by mass | 3D-MoRSE descriptors |  |
| 923 | Mor17m | signal 17 / weighted by mass | 3D-MoRSE descriptors |  |
| 924 | Mor18m | signal 18 / weighted by mass | 3D-MoRSE descriptors |  |
| 925 | Mor19m | signal 19 / weighted by mass | 3D-MoRSE descriptors |  |
| 926 | Mor20m | signal 20 / weighted by mass | 3D-MoRSE descriptors |  |
| 927 | Mor21m | signal 21 / weighted by mass | 3D-MoRSE descriptors |  |
| 928 | Mor22m | signal 22 / weighted by mass | 3D-MoRSE descriptors |  |
| 929 | Mor23m | signal 23 / weighted by mass | 3D-MoRSE descriptors |  |
| 930 | Mor24m | signal 24 / weighted by mass | 3D-MoRSE descriptors |  |
| 931 | Mor25m | signal 25 / weighted by mass | 3D-MoRSE descriptors |  |
| 932 | Mor26m | signal 26 / weighted by mass | 3D-MoRSE descriptors |  |
| 933 | Mor27m | signal 27 / weighted by mass | 3D-MoRSE descriptors |  |
| 934 | Mor28m | signal 28 / weighted by mass | 3D-MoRSE descriptors |  |
| 935 | Mor29m | signal 29 / weighted by mass | 3D-MoRSE descriptors |  |
| 936 | Mor30m | signal 30 / weighted by mass | 3D-MoRSE descriptors |  |
| 937 | Mor31m | signal 31 / weighted by mass | 3D-MoRSE descriptors |  |
| 938 | Mor32m | signal 32 / weighted by mass | 3D-MoRSE descriptors |  |
| 939 | Mor01v | signal 01 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 940 | Mor02v | signal 02 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 941 | Mor03v | signal 03 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 942 | Mor04v | signal 04 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 943 | Mor05v | signal 05 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 944 | Mor06v | signal 06 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 945 | Mor07v | signal 07 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 946 | Mor08v | signal 08 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 947 | Mor09v | signal 09 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 948 | Mor10v | signal 10 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 949 | Mor11v | signal 11 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 950 | Mor12v | signal 12 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 951 | Mor13v | signal 13 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 952 | Mor14v | signal 14 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 953 | Mor15v | signal 15 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 954 | Mor16v | signal 16 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 955 | Mor17v | signal 17 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 956 | Mor18v | signal 18 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 957 | Mor19v | signal 19 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 958 | Mor20v | signal 20 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 959 | Mor21v | signal 21 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 960 | Mor22v | signal 22 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 961 | Mor23v | signal 23 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 962 | Mor24v | signal 24 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 963 | Mor25v | signal 25 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 964 | Mor26v | signal 26 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 965 | Mor27v | signal 27 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 966 | Mor28v | signal 28 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 967 | Mor29v | signal 29 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 968 | Mor30v | signal 30 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 969 | Mor31v | signal 31 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 970 | Mor32v | signal 32 / weighted by van der Waals volume | 3D-MoRSE descriptors |  |
| 971 | Mor01e | signal 01 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 972 | Mor02e | signal 02 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 973 | Mor03e | signal 03 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 974 | Mor04e | signal 04 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 975 | Mor05e | signal 05 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 976 | Mor06e | signal 06 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 977 | Mor07e | signal 07 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 978 | Mor08e | signal 08 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 979 | Mor09e | signal 09 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 980 | Mor10e | signal 10 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 981 | Mor11e | signal 11 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 982 | Mor12e | signal 12 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 983 | Mor13e | signal 13 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 984 | Mor14e | signal 14 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 985 | Mor15e | signal 15 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 986 | Mor16e | signal 16 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 987 | Mor17e | signal 17 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 988 | Mor18e | signal 18 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 989 | Mor19e | signal 19 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 990 | Mor20e | signal 20 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 991 | Mor21e | signal 21 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 992 | Mor22e | signal 22 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 993 | Mor23e | signal 23 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 994 | Mor24e | signal 24 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 995 | Mor25e | signal 25 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 996 | Mor26e | signal 26 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 997 | Mor27e | signal 27 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 998 | Mor28e | signal 28 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 999 | Mor29e | signal 29 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 1000 | Mor30e | signal 30 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 1001 | Mor31e | signal 31 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 1002 | Mor32e | signal 32 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |  |
| 1003 | Mor01p | signal 01 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1004 | Mor02p | signal 02 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1005 | Mor03p | signal 03 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1006 | Mor04p | signal 04 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1007 | Mor05p | signal 05 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1008 | Mor06p | signal 06 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1009 | Mor07p | signal 07 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1010 | Mor08p | signal 08 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1011 | Mor09p | signal 09 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1012 | Mor10p | signal 10 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1013 | Mor11p | signal 11 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1014 | Mor12p | signal 12 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1015 | Mor13p | signal 13 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1016 | Mor14p | signal 14 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1017 | Mor15p | signal 15 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1018 | Mor16p | signal 16 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1019 | Mor17p | signal 17 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1020 | Mor18p | signal 18 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1021 | Mor19p | signal 19 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1022 | Mor20p | signal 20 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1023 | Mor21p | signal 21 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1024 | Mor22p | signal 22 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1025 | Mor23p | signal 23 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1026 | Mor24p | signal 24 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1027 | Mor25p | signal 25 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1028 | Mor26p | signal 26 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1029 | Mor27p | signal 27 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1030 | Mor28p | signal 28 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1031 | Mor29p | signal 29 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1032 | Mor30p | signal 30 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1033 | Mor31p | signal 31 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1034 | Mor32p | signal 32 / weighted by polarizability | 3D-MoRSE descriptors |  |
| 1035 | L1u | 1st component size directional WHIM index / unweighted | WHIM descriptors |  |
| 1036 | L2u | 2nd component size directional WHIM index / unweighted | WHIM descriptors |  |
| 1037 | L3u | 3rd component size directional WHIM index / unweighted | WHIM descriptors |  |
| 1038 | P1u | 1st component shape directional WHIM index / unweighted | WHIM descriptors |  |
| 1039 | P2u | 2nd component shape directional WHIM index / unweighted | WHIM descriptors |  |
| 1040 | G1u | 1st component symmetry directional WHIM index / unweighted | WHIM descriptors |  |
| 1041 | G2u | 2nd component symmetry directional WHIM index / unweighted | WHIM descriptors |  |
| 1042 | G3u | 3rd component symmetry directional WHIM index / unweighted | WHIM descriptors |  |
| 1043 | E1u | 1st component accessibility directional WHIM index / unweighted | WHIM descriptors |  |
| 1044 | E2u | 2nd component accessibility directional WHIM index / unweighted | WHIM descriptors |  |
| 1045 | E3u | 3rd component accessibility directional WHIM index / unweighted | WHIM descriptors |  |
| 1046 | L1m | 1st component size directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1047 | L2m | 2nd component size directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1048 | L3m | 3rd component size directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1049 | P1m | 1st component shape directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1050 | P2m | 2nd component shape directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1051 | G1m | 1st component symmetry directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1052 | G2m | 2nd component symmetry directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1053 | G3m | 3rd component symmetry directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1054 | E1m | 1st component accessibility directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1055 | E2m | 2nd component accessibility directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1056 | E3m | 3rd component accessibility directional WHIM index / weighted by mass | WHIM descriptors |  |
| 1057 | L1v | 1st component size directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1058 | L2v | 2nd component size directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1059 | L3v | 3rd component size directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1060 | P1v | 1st component shape directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1061 | P2v | 2nd component shape directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1062 | G1v | 1st component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1063 | G2v | 2nd component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1064 | G3v | 3rd component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1065 | E1v | 1st component accessibility directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1066 | E2v | 2nd component accessibility directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1067 | E3v | 3rd component accessibility directional WHIM index / weighted by van der Waals volume | WHIM descriptors |  |
| 1068 | L1e | 1st component size directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1069 | L2e | 2nd component size directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1070 | L3e | 3rd component size directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1071 | P1e | 1st component shape directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1072 | P2e | 2nd component shape directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1073 | G1e | 1st component symmetry directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1074 | G2e | 2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1075 | G3e | 3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1076 | E1e | 1st component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1077 | E2e | 2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1078 | E3e | 3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1079 | L1p | 1st component size directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1080 | L2p | 2nd component size directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1081 | L3p | 3rd component size directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1082 | P1p | 1st component shape directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1083 | P2p | 2nd component shape directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1084 | G1p | 1st component symmetry directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1085 | G2p | 2nd component symmetry directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1086 | G3p | 3rd component symmetry directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1087 | E1p | 1st component accessibility directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1088 | E2p | 2nd component accessibility directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1089 | E3p | 3rd component accessibility directional WHIM index / weighted by polarizability | WHIM descriptors |  |
| 1090 | L1s | 1st component size directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1091 | L2s | 2nd component size directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1092 | L3s | 3rd component size directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1093 | P1s | 1st component shape directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1094 | P2s | 2nd component shape directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1095 | G1s | 1st component symmetry directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1096 | G2s | 2nd component symmetry directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1097 | G3s | 3rd component symmetry directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1098 | E1s | 1st component accessibility directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1099 | E2s | 2nd component accessibility directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1100 | E3s | 3rd component accessibility directional WHIM index / weighted by I-state | WHIM descriptors |  |
| 1101 | Tu | T total size index / unweighted | WHIM descriptors |  |
| 1102 | Tm | T total size index / weighted by mass | WHIM descriptors |  |
| 1103 | Tv | T total size index / weighted by van der Waals volume | WHIM descriptors |  |
| 1104 | Te | T total size index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1105 | Tp | T total size index / weighted by polarizability | WHIM descriptors |  |
| 1106 | Ts | T total size index / weighted by I-state | WHIM descriptors |  |
| 1107 | Au | A total size index / unweighted | WHIM descriptors |  |
| 1108 | Am | A total size index / weighted by mass | WHIM descriptors |  |
| 1109 | Av | A total size index / weighted by van der Waals volume | WHIM descriptors |  |
| 1110 | Ae | A total size index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1111 | Ap | A total size index / weighted by polarizability | WHIM descriptors |  |
| 1112 | As | A total size index / weighted by I-state | WHIM descriptors |  |
| 1113 | Gu | total symmetry index / unweighted | WHIM descriptors |  |
| 1114 | Gm | total symmetry index / weighted by mass | WHIM descriptors |  |
| 1115 | Gs | G total symmetry index / weighted by atomic electrotopological states | WHIM descriptors |  |
| 1116 | Ku | K global shape index / unweighted | WHIM descriptors |  |
| 1117 | Km | K global shape index / weighted by mass | WHIM descriptors |  |
| 1118 | Kv | K global shape index / weighted by van der Waals volume | WHIM descriptors |  |
| 1119 | Ke | K global shape index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1120 | Kp | K global shape index / weighted by polarizability | WHIM descriptors |  |
| 1121 | Ks | K global shape index / weighted by I-state | WHIM descriptors |  |
| 1122 | Du | D total accessibility index / unweighted | WHIM descriptors |  |
| 1123 | Dm | D total accessibility index / weighted by mass | WHIM descriptors |  |
| 1124 | Dv | D total accessibility index / weighted by van der Waals volume | WHIM descriptors |  |
| 1125 | De | D total accessibility index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1126 | Dp | D total accessibility index / weighted by polarizability | WHIM descriptors |  |
| 1127 | Ds | D total accessibility index / weighted by I-state | WHIM descriptors |  |
| 1128 | Vu | V total size index / unweighted | WHIM descriptors |  |
| 1129 | Vm | V total size index / weighted by mass | WHIM descriptors |  |
| 1130 | Vv | V total size index / weighted by van der Waals volume | WHIM descriptors |  |
| 1131 | Ve | V total size index / weighted by Sanderson electronegativity | WHIM descriptors |  |
| 1132 | Vp | V total size index / weighted by polarizability | WHIM descriptors |  |
| 1133 | Vs | V total size index / weighted by I-state | WHIM descriptors |  |
| 1134 | ITH | total information content on the leverage equality | GETAWAY descriptors |  |
| 1135 | ISH | standardized information content on the leverage equality | GETAWAY descriptors |  |
| 1136 | HIC | mean information content on the leverage magnitude | GETAWAY descriptors |  |
| 1137 | HGM | geometric mean on the leverage magnitude | GETAWAY descriptors |  |
| 1138 | H0u | H autocorrelation of lag 0 / unweighted | GETAWAY descriptors |  |
| 1139 | H1u | H autocorrelation of lag 1 / unweighted | GETAWAY descriptors |  |
| 1140 | H2u | H autocorrelation of lag 2 / unweighted | GETAWAY descriptors |  |
| 1141 | H3u | H autocorrelation of lag 3 / unweighted | GETAWAY descriptors |  |
| 1142 | H4u | H autocorrelation of lag 4 / unweighted | GETAWAY descriptors |  |
| 1143 | H5u | H autocorrelation of lag 5 / unweighted | GETAWAY descriptors |  |
| 1144 | H6u | H autocorrelation of lag 6 / unweighted | GETAWAY descriptors |  |
| 1145 | H7u | H autocorrelation of lag 7 / unweighted | GETAWAY descriptors |  |
| 1146 | H8u | H autocorrelation of lag 8 / unweighted | GETAWAY descriptors |  |
| 1147 | HTu | H total index / unweighted | GETAWAY descriptors |  |
| 1148 | HATS0u | leverage-weighted autocorrelation of lag 0 / unweighted | GETAWAY descriptors |  |
| 1149 | HATS1u | leverage-weighted autocorrelation of lag 1 / unweighted | GETAWAY descriptors |  |
| 1150 | HATS2u | leverage-weighted autocorrelation of lag 2 / unweighted | GETAWAY descriptors |  |
| 1151 | HATS3u | leverage-weighted autocorrelation of lag 3 / unweighted | GETAWAY descriptors |  |
| 1152 | HATS4u | leverage-weighted autocorrelation of lag 4 / unweighted | GETAWAY descriptors |  |
| 1153 | HATS5u | leverage-weighted autocorrelation of lag 5 / unweighted | GETAWAY descriptors |  |
| 1154 | HATS6u | leverage-weighted autocorrelation of lag 6 / unweighted | GETAWAY descriptors |  |
| 1155 | HATS7u | leverage-weighted autocorrelation of lag 7 / unweighted | GETAWAY descriptors |  |
| 1156 | HATS8u | leverage-weighted autocorrelation of lag 8 / unweighted | GETAWAY descriptors |  |
| 1157 | HATSu | leverage-weighted total index / unweighted | GETAWAY descriptors |  |
| 1158 | H0m | H autocorrelation of lag 0 / weighted by mass | GETAWAY descriptors |  |
| 1159 | H1m | H autocorrelation of lag 1 / weighted by mass | GETAWAY descriptors |  |
| 1160 | H2m | H autocorrelation of lag 2 / weighted by mass | GETAWAY descriptors |  |
| 1161 | H3m | H autocorrelation of lag 3 / weighted by mass | GETAWAY descriptors |  |
| 1162 | H4m | H autocorrelation of lag 4 / weighted by mass | GETAWAY descriptors |  |
| 1163 | H5m | H autocorrelation of lag 5 / weighted by mass | GETAWAY descriptors |  |
| 1164 | H6m | H autocorrelation of lag 6 / weighted by mass | GETAWAY descriptors |  |
| 1165 | H7m | H autocorrelation of lag 7 / weighted by mass | GETAWAY descriptors |  |
| 1166 | H8m | H autocorrelation of lag 8 / weighted by mass | GETAWAY descriptors |  |
| 1167 | HTm | H total index / weighted by mass | GETAWAY descriptors |  |
| 1168 | HATS0m | leverage-weighted autocorrelation of lag 0 / weighted by mass | GETAWAY descriptors |  |
| 1169 | HATS1m | leverage-weighted autocorrelation of lag 1 / weighted by mass | GETAWAY descriptors |  |
| 1170 | HATS2m | leverage-weighted autocorrelation of lag 2 / weighted by mass | GETAWAY descriptors |  |
| 1171 | HATS3m | leverage-weighted autocorrelation of lag 3 / weighted by mass | GETAWAY descriptors |  |
| 1172 | HATS4m | leverage-weighted autocorrelation of lag 4 / weighted by mass | GETAWAY descriptors |  |
| 1173 | HATS5m | leverage-weighted autocorrelation of lag 5 / weighted by mass | GETAWAY descriptors |  |
| 1174 | HATS6m | leverage-weighted autocorrelation of lag 6 / weighted by mass | GETAWAY descriptors |  |
| 1175 | HATS7m | leverage-weighted autocorrelation of lag 7 / weighted by mass | GETAWAY descriptors |  |
| 1176 | HATS8m | leverage-weighted autocorrelation of lag 8 / weighted by mass | GETAWAY descriptors |  |
| 1177 | HATSm | leverage-weighted total index / weighted by mass | GETAWAY descriptors |  |
| 1178 | H0v | H autocorrelation of lag 0 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1179 | H1v | H autocorrelation of lag 1 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1180 | H2v | H autocorrelation of lag 2 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1181 | H3v | H autocorrelation of lag 3 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1182 | H4v | H autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1183 | H5v | H autocorrelation of lag 5 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1184 | H6v | H autocorrelation of lag 6 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1185 | H7v | H autocorrelation of lag 7 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1186 | H8v | H autocorrelation of lag 8 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1187 | HTv | H total index / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1188 | HATS0v | leverage-weighted autocorrelation of lag 0 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1189 | HATS1v | leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1190 | HATS2v | leverage-weighted autocorrelation of lag 2 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1191 | HATS3v | leverage-weighted autocorrelation of lag 3 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1192 | HATS4v | leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1193 | HATS5v | leverage-weighted autocorrelation of lag 5 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1194 | HATS6v | leverage-weighted autocorrelation of lag 6 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1195 | HATS7v | leverage-weighted autocorrelation of lag 7 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1196 | HATS8v | leverage-weighted autocorrelation of lag 8 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1197 | HATSv | leverage-weighted total index / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1198 | H0e | H autocorrelation of lag 0 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1199 | H1e | H autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1200 | H2e | H autocorrelation of lag 2 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1201 | H3e | H autocorrelation of lag 3 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1202 | H4e | H autocorrelation of lag 4 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1203 | H5e | H autocorrelation of lag 5 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1204 | H6e | H autocorrelation of lag 6 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1205 | H7e | H autocorrelation of lag 7 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1206 | H8e | H autocorrelation of lag 8 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1207 | HTe | H total index / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1208 | HATS0e | leverage-weighted autocorrelation of lag 0 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1209 | HATS1e | leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1210 | HATS2e | leverage-weighted autocorrelation of lag 2 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1211 | HATS3e | leverage-weighted autocorrelation of lag 3 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1212 | HATS4e | leverage-weighted autocorrelation of lag 4 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1213 | HATS5e | leverage-weighted autocorrelation of lag 5 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1214 | HATS6e | leverage-weighted autocorrelation of lag 6 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1215 | HATS7e | leverage-weighted autocorrelation of lag 7 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1216 | HATS8e | leverage-weighted autocorrelation of lag 8 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1217 | HATSe | leverage-weighted total index / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1218 | H0p | H autocorrelation of lag 0 / weighted by polarizability | GETAWAY descriptors |  |
| 1219 | H1p | H autocorrelation of lag 1 / weighted by polarizability | GETAWAY descriptors |  |
| 1220 | H2p | H autocorrelation of lag 2 / weighted by polarizability | GETAWAY descriptors |  |
| 1221 | H3p | H autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |  |
| 1222 | H4p | H autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |  |
| 1223 | H5p | H autocorrelation of lag 5 / weighted by polarizability | GETAWAY descriptors |  |
| 1224 | H6p | H autocorrelation of lag 6 / weighted by polarizability | GETAWAY descriptors |  |
| 1225 | H7p | H autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |  |
| 1226 | H8p | H autocorrelation of lag 8 / weighted by polarizability | GETAWAY descriptors |  |
| 1227 | HTp | H total index / weighted by polarizability | GETAWAY descriptors |  |
| 1228 | HATS0p | leverage-weighted autocorrelation of lag 0 / weighted by polarizability | GETAWAY descriptors |  |
| 1229 | HATS1p | leverage-weighted autocorrelation of lag 1 / weighted by polarizability | GETAWAY descriptors |  |
| 1230 | HATS2p | leverage-weighted autocorrelation of lag 2 / weighted by polarizability | GETAWAY descriptors |  |
| 1231 | HATS3p | leverage-weighted autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |  |
| 1232 | HATS4p | leverage-weighted autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |  |
| 1233 | HATS5p | leverage-weighted autocorrelation of lag 5 / weighted by polarizability | GETAWAY descriptors |  |
| 1234 | HATS6p | leverage-weighted autocorrelation of lag 6 / weighted by polarizability | GETAWAY descriptors |  |
| 1235 | HATS7p | leverage-weighted autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |  |
| 1236 | HATS8p | leverage-weighted autocorrelation of lag 8 / weighted by polarizability | GETAWAY descriptors |  |
| 1237 | HATSp | leverage-weighted total index / weighted by polarizability | GETAWAY descriptors |  |
| 1238 | RCON | Randic-type R matrix connectivity | GETAWAY descriptors |  |
| 1239 | RARS | R matrix average row sum | GETAWAY descriptors |  |
| 1240 | REIG | first eigenvalue of the R matrix | GETAWAY descriptors |  |
| 1241 | R1u | R autocorrelation of lag 1 / unweighted | GETAWAY descriptors |  |
| 1242 | R2u | R autocorrelation of lag 2 / unweighted | GETAWAY descriptors |  |
| 1243 | R3u | R autocorrelation of lag 3 / unweighted | GETAWAY descriptors |  |
| 1244 | R4u | R autocorrelation of lag 4 / unweighted | GETAWAY descriptors |  |
| 1245 | R5u | R autocorrelation of lag 5 / unweighted | GETAWAY descriptors |  |
| 1246 | R6u | R autocorrelation of lag 6 / unweighted | GETAWAY descriptors |  |
| 1247 | R7u | R autocorrelation of lag 7 / unweighted | GETAWAY descriptors |  |
| 1248 | R8u | R autocorrelation of lag 8 / unweighted | GETAWAY descriptors |  |
| 1249 | RTu | R total index / unweighted | GETAWAY descriptors |  |
| 1250 | R1u+ | R maximal autocorrelation of lag 1 / unweighted | GETAWAY descriptors |  |
| 1251 | R2u+ | R maximal autocorrelation of lag 2 / unweighted | GETAWAY descriptors |  |
| 1252 | R3u+ | R maximal autocorrelation of lag 3 / unweighted | GETAWAY descriptors |  |
| 1253 | R4u+ | R maximal autocorrelation of lag 4 / unweighted | GETAWAY descriptors |  |
| 1254 | R5u+ | R maximal autocorrelation of lag 5 / unweighted | GETAWAY descriptors |  |
| 1255 | R6u+ | R maximal autocorrelation of lag 6 / unweighted | GETAWAY descriptors |  |
| 1256 | R7u+ | R maximal autocorrelation of lag 7 / unweighted | GETAWAY descriptors |  |
| 1257 | R8u+ | R maximal autocorrelation of lag 8 / unweighted | GETAWAY descriptors |  |
| 1258 | RTu+ | R maximal index / unweighted | GETAWAY descriptors |  |
| 1259 | R1m | R autocorrelation of lag 1 / weighted by mass | GETAWAY descriptors |  |
| 1260 | R2m | R autocorrelation of lag 2 / weighted by mass | GETAWAY descriptors |  |
| 1261 | R3m | R autocorrelation of lag 3 / weighted by mass | GETAWAY descriptors |  |
| 1262 | R4m | R autocorrelation of lag 4 / weighted by mass | GETAWAY descriptors |  |
| 1263 | R5m | R autocorrelation of lag 5 / weighted by mass | GETAWAY descriptors |  |
| 1264 | R6m | R autocorrelation of lag 6 / weighted by mass | GETAWAY descriptors |  |
| 1265 | R7m | R autocorrelation of lag 7 / weighted by mass | GETAWAY descriptors |  |
| 1266 | R8m | R autocorrelation of lag 8 / weighted by mass | GETAWAY descriptors |  |
| 1267 | RTm | R total index / weighted by mass | GETAWAY descriptors |  |
| 1268 | R1m+ | R maximal autocorrelation of lag 1 / weighted by mass | GETAWAY descriptors |  |
| 1269 | R2m+ | R maximal autocorrelation of lag 2 / weighted by mass | GETAWAY descriptors |  |
| 1270 | R3m+ | R maximal autocorrelation of lag 3 / weighted by mass | GETAWAY descriptors |  |
| 1271 | R4m+ | R maximal autocorrelation of lag 4 / weighted by mass | GETAWAY descriptors |  |
| 1272 | R5m+ | R maximal autocorrelation of lag 5 / weighted by mass | GETAWAY descriptors |  |
| 1273 | R6m+ | R maximal autocorrelation of lag 6 / weighted by mass | GETAWAY descriptors |  |
| 1274 | R7m+ | R maximal autocorrelation of lag 7 / weighted by mass | GETAWAY descriptors |  |
| 1275 | R8m+ | R maximal autocorrelation of lag 8 / weighted by mass | GETAWAY descriptors |  |
| 1276 | RTm+ | R maximal index / weighted by mass | GETAWAY descriptors |  |
| 1277 | R1v | R autocorrelation of lag 1 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1278 | R2v | R autocorrelation of lag 2 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1279 | R3v | R autocorrelation of lag 3 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1280 | R4v | R autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1281 | R5v | R autocorrelation of lag 5 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1282 | R6v | R autocorrelation of lag 6 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1283 | R7v | R autocorrelation of lag 7 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1284 | R8v | R autocorrelation of lag 8 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1285 | RTv | R total index / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1286 | R1v+ | R maximal autocorrelation of lag 1 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1287 | R2v+ | R maximal autocorrelation of lag 2 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1288 | R3v+ | R maximal autocorrelation of lag 3 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1289 | R4v+ | R maximal autocorrelation of lag 4 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1290 | R5v+ | R maximal autocorrelation of lag 5 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1291 | R6v+ | R maximal autocorrelation of lag 6 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1292 | R7v+ | R maximal autocorrelation of lag 7 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1293 | R8v+ | R maximal autocorrelation of lag 8 / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1294 | RTv+ | R maximal index / weighted by van der Waals volume | GETAWAY descriptors |  |
| 1295 | R1e | R autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1296 | R2e | R autocorrelation of lag 2 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1297 | R3e | R autocorrelation of lag 3 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1298 | R4e | R autocorrelation of lag 4 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1299 | R5e | R autocorrelation of lag 5 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1300 | R6e | R autocorrelation of lag 6 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1301 | R7e | R autocorrelation of lag 7 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1302 | R8e | R autocorrelation of lag 8 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1303 | RTe | R total index / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1304 | R1e+ | R maximal autocorrelation of lag 1 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1305 | R2e+ | R maximal autocorrelation of lag 2 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1306 | R3e+ | R maximal autocorrelation of lag 3 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1307 | R4e+ | R maximal autocorrelation of lag 4 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1308 | R5e+ | R maximal autocorrelation of lag 5 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1309 | R6e+ | R maximal autocorrelation of lag 6 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1310 | R7e+ | R maximal autocorrelation of lag 7 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1311 | R8e+ | R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1312 | RTe+ | R maximal index / weighted by Sanderson electronegativity | GETAWAY descriptors |  |
| 1313 | R1p | R autocorrelation of lag 1 / weighted by polarizability | GETAWAY descriptors |  |
| 1314 | R2p | R autocorrelation of lag 2 / weighted by polarizability | GETAWAY descriptors |  |
| 1315 | R3p | R autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |  |
| 1316 | R4p | R autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |  |
| 1317 | R5p | R autocorrelation of lag 5 / weighted by polarizability | GETAWAY descriptors |  |
| 1318 | R6p | R autocorrelation of lag 6 / weighted by polarizability | GETAWAY descriptors |  |
| 1319 | R7p | R autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |  |
| 1320 | R8p | R autocorrelation of lag 8 / weighted by polarizability | GETAWAY descriptors |  |
| 1321 | RTp | R total index / weighted by polarizability | GETAWAY descriptors |  |
| 1322 | R1p+ | R maximal autocorrelation of lag 1 / weighted by polarizability | GETAWAY descriptors |  |
| 1323 | R2p+ | R maximal autocorrelation of lag 2 / weighted by polarizability | GETAWAY descriptors |  |
| 1324 | R3p+ | R maximal autocorrelation of lag 3 / weighted by polarizability | GETAWAY descriptors |  |
| 1325 | R4p+ | R maximal autocorrelation of lag 4 / weighted by polarizability | GETAWAY descriptors |  |
| 1326 | R5p+ | R maximal autocorrelation of lag 5 / weighted by polarizability | GETAWAY descriptors |  |
| 1327 | R6p+ | R maximal autocorrelation of lag 6 / weighted by polarizability | GETAWAY descriptors |  |
| 1328 | R7p+ | R maximal autocorrelation of lag 7 / weighted by polarizability | GETAWAY descriptors |  |
| 1329 | R8p+ | R maximal autocorrelation of lag 8 / weighted by polarizability | GETAWAY descriptors |  |
| 1330 | RTp+ | R maximal index / weighted by polarizability | GETAWAY descriptors |  |
| 1331 | nCp | number of terminal primary C(sp3) | Functional group counts |  |
| 1332 | nCs | number of total secondary C(sp3) | Functional group counts |  |
| 1333 | nCt | number of total tertiary C(sp3) | Functional group counts |  |
| 1334 | nCq | number of total quaternary C(sp3) | Functional group counts |  |
| 1335 | nCrs | number of ring secondary C(sp3) | Functional group counts |  |
| 1336 | nCrt | number of ring tertiary C(sp3) | Functional group counts |  |
| 1337 | nCrq | number of ring quaternary C(sp3) | Functional group counts |  |
| 1338 | nCar | number of aromatic C(sp2) | Functional group counts |  |
| 1339 | nCbH | number of unsubstituted benzene C(sp2) | Functional group counts |  |
| 1340 | nCb- | number of substituted benzene C(sp2) | Functional group counts |  |
| 1341 | nCconj | number of non-aromatic conjugated C(sp2) | Functional group counts |  |
| 1342 | nR=Cp | number of terminal primary C(sp2) | Functional group counts |  |
| 1343 | nR=Cs | number of aliphatic secondary C(sp2) | Functional group counts |  |
| 1344 | nR=Ct | number of aliphatic tertiary C(sp2) | Functional group counts |  |
| 1345 | nR#CH/X | number of terminal C(sp) | Functional group counts |  |
| 1346 | nR#C- | number of non-terminal C(sp) | Functional group counts |  |
| 1347 | nArNCO | number of cyanates (aliphatic) | Functional group counts |  |
| 1348 | nRSCN | number of thiocyanates (aliphatic) | Functional group counts |  |
| 1349 | nRNCS | number of isothiocyanates (aliphatic) | Functional group counts |  |
| 1350 | nArNCS | number of isothiocyanates (aromatic) | Functional group counts |  |
| 1351 | nRCOOH | number of carboxylic acids (aliphatic) | Functional group counts |  |
| 1352 | nArCOOH | number of carboxylic acids (aromatic) | Functional group counts |  |
| 1353 | nRCOOR | number of esters (aliphatic) | Functional group counts |  |
| 1354 | nArCOOR | number of esters (aromatic) | Functional group counts |  |
| 1355 | nRCONH2 | number of primary amides (aliphatic) | Functional group counts |  |
| 1356 | nArCONH2 | number of primary amides (aromatic) | Functional group counts |  |
| 1357 | nRCONHR | number of secondary amides (aliphatic) | Functional group counts |  |
| 1358 | nArCONHR | number of secondary amides (aromatic) | Functional group counts |  |
| 1359 | nRCONR2 | number of tertiary amides (aliphatic) | Functional group counts |  |
| 1360 | nArCONR2 | number of tertiary amides (aromatic) | Functional group counts |  |
| 1361 | nROCON | number of (thio-) carbamates (aliphatic) | Functional group counts |  |
| 1362 | nArOCON | number of (thio-) carbamates (aromatic) | Functional group counts |  |
| 1363 | nRCOX | number of acyl halogenides (aliphatic) | Functional group counts |  |
| 1364 | nArCOX | number of acyl halogenides (aromatic) | Functional group counts |  |
| 1365 | nRCHO | number of aldehydes (aliphatic) | Functional group counts |  |
| 1366 | nArCHO | number of aldehydes (aromatic) | Functional group counts |  |
| 1367 | nRCO | number of ketones (aliphatic) | Functional group counts |  |
| 1368 | nArCO | number of ketones (aromatic) | Functional group counts |  |
| 1369 | nCONN | number of urea (-thio) derivatives | Functional group counts |  |
| 1370 | nC=O(O)2 | number of carbonate (-thio) derivatives | Functional group counts |  |
| 1371 | nN=C-N< | number of amidine derivatives | Functional group counts |  |
| 1372 | nC(=N)N2 | number of guanidine derivatives | Functional group counts |  |
| 1373 | nRC=N | number of imines (aliphatic) | Functional group counts |  |
| 1374 | nArC=N | number of imines (aromatic) | Functional group counts |  |
| 1375 | nRCNO | number of oximes (aliphatic) | Functional group counts |  |
| 1376 | nArCNO | number of oximes (aromatic) | Functional group counts |  |
| 1377 | nRNH2 | number of primary amines (aliphatic) | Functional group counts |  |
| 1378 | nArNH2 | number of primary amines (aromatic) | Functional group counts |  |
| 1379 | nRNHR | number of secondary amines (aliphatic) | Functional group counts |  |
| 1380 | nArNHR | number of secondary amines (aromatic) | Functional group counts |  |
| 1381 | nRNR2 | number of tertiary amines (aliphatic) | Functional group counts |  |
| 1382 | nArNR2 | number of tertiary amines (aromatic) | Functional group counts |  |
| 1383 | nN-N | number of N hydrazines | Functional group counts |  |
| 1384 | nN=N | number of N azo-derivatives | Functional group counts |  |
| 1385 | nRCN | number of nitriles (aliphatic) | Functional group counts |  |
| 1386 | nArCN | number of nitriles (aromatic) | Functional group counts |  |
| 1387 | nN+ | number of positively charged N | Functional group counts |  |
| 1388 | nNq | number of quaternary N | Functional group counts |  |
| 1389 | nRNHO | number of hydroxylamines (aliphatic) | Functional group counts |  |
| 1390 | nArNHO | number of hydroxylamines (aromatic) | Functional group counts |  |
| 1391 | nRNNOx | number of N-nitroso groups (aliphatic) | Functional group counts |  |
| 1392 | nArNNOx | number of N-nitroso groups (aromatic) | Functional group counts |  |
| 1393 | nArNO | number of nitroso groups (aromatic) | Functional group counts |  |
| 1394 | nRNO2 | number of nitro groups (aliphatic) | Functional group counts |  |
| 1395 | nArNO2 | number of nitro groups (aromatic) | Functional group counts |  |
| 1396 | nN(CO)2 | number of imides (-thio) | Functional group counts |  |
| 1397 | nC=N-N< | number of hydrazones | Functional group counts |  |
| 1398 | nROH | number of hydroxyl groups | Functional group counts |  |
| 1399 | nArOH | number of aromatic hydroxyls | Functional group counts |  |
| 1400 | nOHp | number of primary alcohols | Functional group counts |  |
| 1401 | nOHs | number of secondary alcohols | Functional group counts |  |
| 1402 | nOHt | number of tertiary alcohols | Functional group counts |  |
| 1403 | nROR | number of ethers (aliphatic) | Functional group counts |  |
| 1404 | nArOR | number of ethers (aromatic) | Functional group counts |  |
| 1405 | nO(C=O)2 | number of anhydrides (-thio) | Functional group counts |  |
| 1406 | nSH | number of thiols | Functional group counts |  |
| 1407 | nRSR | number of sulfides | Functional group counts |  |
| 1408 | nRSSR | number of disulfides | Functional group counts |  |
| 1409 | nSO | number of sulfoxides | Functional group counts |  |
| 1410 | nS(=O)2 | number of sulfones | Functional group counts |  |
| 1411 | nSO2OH | number of sulfonic (thio-/dithio-) acids | Functional group counts |  |
| 1412 | nSO3OH | number of sulfuric (thio-/dithio-) acids | Functional group counts |  |
| 1413 | nSO3 | number of sulfonates (thio-/dithio-) | Functional group counts |  |
| 1414 | nSO4 | number of sulfates (thio-/dithio-) | Functional group counts |  |
| 1415 | nSO2N | number of sulfonamides (thio-/dithio-) | Functional group counts |  |
| 1416 | nPO3 | number of phosphites/thiophosphites | Functional group counts |  |
| 1417 | nPO4 | number of phosphates/thiophosphates | Functional group counts |  |
| 1418 | nP(=O)O2R | number of phosphonates (thio-) | Functional group counts |  |
| 1419 | nCH2RX | number of CH2RX | Functional group counts |  |
| 1420 | nCHR2X | number of CHR2X | Functional group counts |  |
| 1421 | nCR3X | number of CR3X | Functional group counts |  |
| 1422 | nR=CHX | number of R=CHX | Functional group counts |  |
| 1423 | nR=CRX | number of R=CRX | Functional group counts |  |
| 1424 | nCHRX2 | number of CHRX2 | Functional group counts |  |
| 1425 | nCR2X2 | number of CR2X2 | Functional group counts |  |
| 1426 | nR=CX2 | number of R=CX2 | Functional group counts |  |
| 1427 | nCRX3 | number of CRX3 | Functional group counts |  |
| 1428 | nArX | number of X on aromatic ring | Functional group counts |  |
| 1429 | nCXr | number of X on ring C(sp3) | Functional group counts |  |
| 1430 | nCXr= | number of X on ring C(sp2) | Functional group counts |  |
| 1431 | nCconjX | number of X on exo-conjugated C | Functional group counts |  |
| 1432 | nAziridines | number of Aziridines | Functional group counts |  |
| 1433 | nOxiranes | number of Oxiranes | Functional group counts |  |
| 1434 | nThiranes | number of Thiranes | Functional group counts |  |
| 1435 | nOxetanes | number of Oxetanes | Functional group counts |  |
| 1436 | nBeta-Lactams | number of Beta-Lactams | Functional group counts |  |
| 1437 | nPyrrolidines | number of Pyrrolidines | Functional group counts |  |
| 1438 | nOxolanes | number of Oxolanes | Functional group counts |  |
| 1439 | ntH-Thiophenes | number of tetrahydro-thiophenes | Functional group counts |  |
| 1440 | nPyrroles | number of Pyrroles | Functional group counts |  |
| 1441 | nPyrazoles | number of Pyrazoles | Functional group counts |  |
| 1442 | nImidazoles | number of Imidazoles | Functional group counts |  |
| 1443 | nFuranes | number of Furanes | Functional group counts |  |
| 1444 | nThiophenes | number of Thiophenes | Functional group counts |  |
| 1445 | nOxazoles | number of Oxazoles | Functional group counts |  |
| 1446 | nIsoxazoles | number of Isoxazoles | Functional group counts |  |
| 1447 | nThiazoles | number of Thiazoles | Functional group counts |  |
| 1448 | nIsothiazoles | number of Isothiazoles | Functional group counts |  |
| 1449 | nTriazoles | number of Triazoles | Functional group counts |  |
| 1450 | nPyridines | number of Pyridines | Functional group counts |  |
| 1451 | nPyridazines | number of Pyridazines | Functional group counts |  |
| 1452 | nPyrimidines | number of Pyrimidines | Functional group counts |  |
| 1453 | nPyrazines | number of Pyrazines | Functional group counts |  |
| 1454 | n135-Triazines | number of 1-3-5-Triazines | Functional group counts |  |
| 1455 | nHDon | number of donor atoms for H-bonds (N and O) | Functional group counts |  |
| 1456 | nHAcc | number of acceptor atoms for H-bonds (N,O,F) | Functional group counts |  |
| 1457 | nHBonds | number of intramolecular H-bonds (with N,O,F) | Functional group counts |  |
| 1458 | C-001 | CH3R, CH4 | Atom-centred fragments |  |
| 1459 | C-002 | CH2R2 | Atom-centred fragments |  |
| 1460 | C-003 | CHR3 | Atom-centred fragments |  |
| 1461 | C-004 | CR4 | Atom-centred fragments |  |
| 1462 | C-005 | CH3X | Atom-centred fragments |  |
| 1463 | C-006 | CH2RX | Atom-centred fragments |  |
| 1464 | C-007 | CH2X2 | Atom-centred fragments |  |
| 1465 | C-008 | CHR2X | Atom-centred fragments |  |
| 1466 | C-009 | CHRX2 | Atom-centred fragments |  |
| 1467 | C-011 | CR3X | Atom-centred fragments |  |
| 1468 | C-012 | CR2X2 | Atom-centred fragments |  |
| 1469 | C-013 | CRX3 | Atom-centred fragments |  |
| 1470 | C-014 | CX4 | Atom-centred fragments |  |
| 1471 | C-015 | #REF! | Atom-centred fragments |  |
| 1472 | C-016 | #NAME? | Atom-centred fragments |  |
| 1473 | C-017 | #REF! | Atom-centred fragments |  |
| 1474 | C-018 | #NAME? | Atom-centred fragments |  |
| 1475 | C-019 | #NAME? | Atom-centred fragments |  |
| 1476 | C-020 | #REF! | Atom-centred fragments |  |
| 1477 | C-021 | ≡CH | Atom-centred fragments |  |
| 1478 | C-022 | ≡CR, R=C=R | Atom-centred fragments |  |
| 1479 | C-024 | R:CH:R | Atom-centred fragments |  |
| 1480 | C-025 | R:CR:R | Atom-centred fragments |  |
| 1481 | C-026 | R:CX:R | Atom-centred fragments |  |
| 1482 | C-027 | R:CH:X | Atom-centred fragments |  |
| 1483 | C-028 | R:CR:X | Atom-centred fragments |  |
| 1484 | C-029 | R:CX:X | Atom-centred fragments |  |
| 1485 | C-030 | X:CH:X | Atom-centred fragments |  |
| 1486 | C-031 | X:CR:X | Atom-centred fragments |  |
| 1487 | C-032 | X:CX:X | Atom-centred fragments |  |
| 1488 | C-033 | R:CH•••X | Atom-centred fragments |  |
| 1489 | C-034 | R:CR•••X | Atom-centred fragments |  |
| 1490 | C-035 | R:CX•••X | Atom-centred fragments |  |
| 1491 | C-036 | Al-CH=X | Atom-centred fragments |  |
| 1492 | C-037 | Ar-CH=X | Atom-centred fragments |  |
| 1493 | C-038 | Al-C(=X)-Al | Atom-centred fragments |  |
| 1494 | C-039 | Ar-C(=X)-R | Atom-centred fragments |  |
| 1495 | C-040 | R-C(=X)-X, R-C≡X, X=C=X | Atom-centred fragments |  |
| 1496 | C-041 | X-C(=X)-X | Atom-centred fragments |  |
| 1497 | C-042 | X:CH•••X | Atom-centred fragments |  |
| 1498 | C-043 | X:CR•••X | Atom-centred fragments |  |
| 1499 | C-044 | X:CX•••X | Atom-centred fragments |  |
| 1500 | H-046 | H attached to C0sp3 no X attached to next C | Atom-centred fragments |  |
| 1501 | H-047 | H attached to C1sp3, C0sp2 | Atom-centred fragments |  |
| 1502 | H-048 | H attached to C2sp3, C1sp2, C0sp | Atom-centred fragments |  |
| 1503 | H-049 | H attached to C3sp3, C2-3sp2, C3sp | Atom-centred fragments |  |
| 1504 | H-050 | H attached to heteroatom | Atom-centred fragments |  |
| 1505 | H-051 | H attached to α-C | Atom-centred fragments |  |
| 1506 | H-052 | H attached to C0sp3 with 1X attached to next C | Atom-centred fragments |  |
| 1507 | H-053 | H attached to C0sp3 with 2X attached to next C | Atom-centred fragments |  |
| 1508 | H-054 | H attached to C0sp3 with 3X attached to next C | Atom-centred fragments |  |
| 1509 | O-056 | alcohol | Atom-centred fragments |  |
| 1510 | O-057 | phenol, enol, carboxyl OH | Atom-centred fragments |  |
| 1511 | O-058 | #NAME? | Atom-centred fragments |  |
| 1512 | O-059 | Al-O-Al | Atom-centred fragments |  |
| 1513 | O-060 | Al-O-Ar, Ar-O-Ar, R•••O•••R, R-O-C=X | Atom-centred fragments |  |
| 1514 | O-061 | -O (as in nitro, N-oxide) | Atom-centred fragments |  |
| 1515 | O-062 | O– (negatively charged) | Atom-centred fragments |  |
| 1516 | O-063 | R-O-O-R | Atom-centred fragments |  |
| 1517 | N-066 | Al-NH2 | Atom-centred fragments |  |
| 1518 | N-067 | Al2-NH | Atom-centred fragments |  |
| 1519 | N-068 | Al3-N | Atom-centred fragments |  |
| 1520 | N-069 | Ar-NH2, X-NH2 | Atom-centred fragments |  |
| 1521 | N-070 | Ar-NH-Al | Atom-centred fragments |  |
| 1522 | N-071 | Ar-NAl2 | Atom-centred fragments |  |
| 1523 | N-072 | RCO-N<, >N-X=X | Atom-centred fragments |  |
| 1524 | N-073 | Ar2NH, Ar3N, Ar2N-Al, R•••N•••R (pyrrole-type structure) | Atom-centred fragments |  |
| 1525 | N-074 | R≡N, R=N- | Atom-centred fragments |  |
| 1526 | N-075 | R:N:R, R:N:X (pyridine-type structure) | Atom-centred fragments |  |
| 1527 | N-076 | Ar-NO2, R:N(:R):O (pyridine N-oxide type structure), RO-NO | Atom-centred fragments |  |
| 1528 | N-077 | Al-NO2 | Atom-centred fragments |  |
| 1529 | N-078 | Ar-N=X, X-N=X | Atom-centred fragments |  |
| 1530 | N-079 | N+ (positively charged) | Atom-centred fragments |  |
| 1531 | F-081 | F attached to C1sp3 | Atom-centred fragments |  |
| 1532 | F-082 | F attached to C22sp3 | Atom-centred fragments |  |
| 1533 | F-083 | F attached to C3sp3 | Atom-centred fragments |  |
| 1534 | F-084 | F attached to C1sp2 | Atom-centred fragments |  |
| 1535 | F-085 | F attached to C2-4sp2, C1sp, C4sp3, X | Atom-centred fragments |  |
| 1536 | Cl-086 | Cl attached to C1sp3 | Atom-centred fragments |  |
| 1537 | Cl-087 | Cl attached to C2sp3 | Atom-centred fragments |  |
| 1538 | Cl-088 | Cl attached to C3sp3 | Atom-centred fragments |  |
| 1539 | Cl-089 | Cl attached to C1sp2 | Atom-centred fragments |  |
| 1540 | Cl-090 | Cl attached to C2-4sp2, C1sp, C4sp3, X | Atom-centred fragments |  |
| 1541 | Br-091 | Br attached to C1sp3 | Atom-centred fragments |  |
| 1542 | Br-092 | Br attached to C2sp3 | Atom-centred fragments |  |
| 1543 | Br-094 | Br attached to C1sp2 | Atom-centred fragments |  |
| 1544 | Br-095 | Br attached to C2-4sp2, C1sp, C4sp3, X | Atom-centred fragments |  |
| 1545 | I-096 | I attached to C1sp3 | Atom-centred fragments |  |
| 1546 | I-099 | I attached to C1sp2 | Atom-centred fragments |  |
| 1547 | S-106 | R-SH | Atom-centred fragments |  |
| 1548 | S-107 | R2S, RS-SR | Atom-centred fragments |  |
| 1549 | S-108 | R=S | Atom-centred fragments |  |
| 1550 | S-109 | R-SO-R | Atom-centred fragments |  |
| 1551 | S-110 | R-SO2-R | Atom-centred fragments |  |
| 1552 | P-117 | X3-P=X (phosphate) | Atom-centred fragments |  |
| 1553 | P-118 | PX3 (phosphite) | Atom-centred fragments |  |
| 1554 | P-120 | C-P(X)2=X (phosphonate) | Atom-centred fragments |  |
| 1555 | qpmax | maximum positive charge | Charge descriptors |  |
| 1556 | qnmax | maximum negative charge | Charge descriptors |  |
| 1557 | Qpos | total positive charge | Charge descriptors |  |
| 1558 | Qneg | total negative charge | Charge descriptors |  |
| 1559 | Qtot | total absolute charge (electronic charge index – ECI) | Charge descriptors |  |
| 1560 | Qmean | mean absolute charge (charge polarization) | Charge descriptors |  |
| 1561 | Q2 | total squared charge | Charge descriptors |  |
| 1562 | RPCG | relative positive charge | Charge descriptors |  |
| 1563 | RNCG | relative negative charge | Charge descriptors |  |
| 1564 | SPP | submolecular polarity parameter | Charge descriptors |  |
| 1565 | TE1 | topographic electronic descriptor | Charge descriptors |  |
| 1566 | TE2 | topographic electronic descriptor (bond resctricted) | Charge descriptors |  |
| 1567 | PCWTE1 | partial charge weighted topological electronic index | Charge descriptors |  |
| 1568 | LDI | local dipole index | Charge descriptors |  |
| 1569 | Ui | unsaturation index | Molecular properties |  |
| 1570 | Hy | hydrophilic factor | Molecular properties |  |
| 1571 | AMR | Ghose-Crippen molar refractivity | Molecular properties |  |
| 1572 | TPSA(NO) | topological polar surface area using N,O polar contributions | Molecular properties |  |
| 1573 | TPSA(Tot) | topological polar surface area using N,O,S,P polar contributions | Molecular properties |  |
| 1574 | MLOGP | Moriguchi octanol-water partition coeff. (logP) | Molecular properties |  |
| 1575 | MLOGP2 | squared Moriguchi octanol-water partition coeff. (logP^2) | Molecular properties |  |
| 1576 | ALOGP | Ghose-Crippen octanol-water partition coeff. (logP) | Molecular properties |  |
| 1577 | ALOGP2 | squared Ghose-Crippen octanol-water partition coeff. (logP^2) | Molecular properties |  |
| 1578 | cRo5 | Drug-like indices | Basic indices |  |
| 1579 | CMC-80 | Drug-like indices | Basic indices |  |
| 1580 | CMC-50 | Drug-like indices | Basic indices |  |
| 1581 | Inflammat-80 | Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80% | Drug-like indices |  |
| 1582 | Inflammat-50 | Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50% | Drug-like indices |  |
| 1583 | Depressant-80 | Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80% | Drug-like indices |  |
| 1584 | Depressant-50 | Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50% | Drug-like indices |  |
| 1585 | Psychotic-80 | Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80% | Drug-like indices |  |
| 1586 | Psychotic-50 | Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50% | Drug-like indices |  |
| 1587 | Hypertens-80 | Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80% | Drug-like indices |  |
| 1588 | Hypertens-50 | Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50% | Drug-like indices |  |
| 1589 | Hypnotic-80 | Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80% | Drug-like indices |  |
| 1590 | Hypnotic-50 | Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50% | Drug-like indices |  |
| 1591 | Neoplastic-80 | Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80% | Drug-like indices |  |
| 1592 | Neoplastic-50 | Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50% | Drug-like indices |  |
| 1593 | Infective-80 | Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80% | Drug-like indices |  |
| 1594 | Infective-50 | Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50% | Drug-like indices |  |
| 1595 | BLTF97 | Verhaar Fish base-line toxicity from MLOGP (mmol/l) | Molecular properties |  |
| 1596 | BLTD49 | Verhaar Daphnia base-line toxicity from MLOGP (mmol/l) | Molecular properties |  |
| 1597 | BLTA97 | Verhaar Algae base-line toxicity from MLOGP (mmol/l) | Molecular properties |  |

**Supplementary 3**: ROC and Precision-Recall curves of the traditional machine learning methods for mutagenicity prediction (page no. 155-159)

|  |  |  |  |
| --- | --- | --- | --- |
| **ML Method** | **Feature reduction by PCA** | **ROC** | **Precision-Recall curve** |
| SVM (sigmoid) | No |  |  |
| SVM (linear) | No |  |  |
| SVM (polynomial) | No |  |  |
| SVM (RBF) | No |  |  |
| RF | No |  |  |
| KNN | No |  |  |
| SVM (sigmoid) | Yes |  |  |
| SVM (linear) | Yes |  |  |
| SVM (Polynomial) | Yes |  |  |
| SVM (RBF) | Yes |  |  |
| RF | Yes |  |  |
| k-NN | Yes |  |  |