**Table S1.** The Molecular Orbital Coefficients of 4-(5-Phenyl-1,3,4-oxadiazol-2-ylthio)-3-methylbenzene-1,2diol (POTMBD) using B3LYP/6-31G(d) method.

74 75 76 77 78

O O O O O

Eigenvalues -- -0.26720 -0.25991 -0.24907 -0.22531 -0.22208

1 1 C 1S 0.00037 -0.00006 0.00024 -0.00006 0.00022

2 2S -0.00076 0.00021 -0.00108 -0.00023 -0.00039

3 2PX 0.02949 0.00088 0.00502 -0.00834 -0.02036

4 2PY -0.01876 -0.00025 -0.00468 0.00542 0.01186

5 2PZ -0.23961 -0.00555 -0.03382 0.06727 0.17077

6 3S -0.00138 -0.00117 0.00911 0.00687 -0.00144

7 3PX 0.01898 0.00028 0.00557 -0.00262 -0.01720

8 3PY -0.01272 -0.00085 0.00175 0.00645 0.00955

9 3PZ -0.16810 -0.00417 -0.02511 0.05205 0.13265

10 4XX 0.00051 -0.00307 0.00007 -0.00001 -0.00032

11 4YY -0.00046 -0.00140 0.00013 -0.00004 0.00014

12 4ZZ 0.00001 0.00444 -0.00008 0.00006 0.00023

13 4XY 0.00023 0.00236 0.00009 -0.00001 0.00002

14 4XZ -0.00223 0.01443 -0.00030 0.00067 0.00139

15 4YZ -0.00348 -0.01076 -0.00036 0.00022 0.00059

16 2 C 1S 0.00014 0.00003 0.00030 -0.00008 0.00019

17 2S -0.00046 -0.00006 -0.00032 0.00071 -0.00055

18 2PX 0.01378 -0.03454 0.00123 -0.00361 -0.00908

19 2PY -0.01001 0.02061 -0.00172 0.00250 0.00420

20 2PZ -0.12465 0.28685 -0.01646 0.03064 0.07222

21 3S 0.00203 0.00073 -0.01143 -0.00840 0.00131

22 3PX 0.00901 -0.02503 0.00350 0.00216 -0.00833

23 3PY -0.00596 0.01551 -0.00799 -0.00466 0.00463

24 3PZ -0.08844 0.20306 -0.01043 0.02452 0.05386

25 4XX -0.00226 -0.00143 -0.00030 0.00067 0.00181

26 4YY 0.00037 0.00098 -0.00009 -0.00029 -0.00030

27 4ZZ 0.00193 0.00048 0.00031 -0.00050 -0.00142

28 4XY 0.00048 -0.00043 0.00014 -0.00015 -0.00025

29 4XZ 0.01071 0.00708 0.00163 -0.00342 -0.00885

30 4YZ 0.00250 0.00793 0.00058 -0.00131 -0.00364

31 3 C 1S 0.00024 -0.00012 -0.00029 0.00048 -0.00017

32 2S -0.00051 0.00021 0.00106 -0.00090 0.00048

33 2PX -0.01292 -0.03467 -0.00003 0.00465 0.01344

34 2PY 0.00817 0.02130 0.00131 -0.00370 -0.00689

35 2PZ 0.10701 0.29524 0.01955 -0.04380 -0.11735

36 3S -0.00528 0.00047 -0.00229 0.00343 -0.00401

37 3PX -0.00669 -0.02315 -0.01807 -0.01282 0.01435

38 3PY 0.00514 0.01494 -0.00301 0.00137 -0.00814

39 3PZ 0.07508 0.21233 0.01068 -0.03889 -0.09393

40 4XX 0.00032 0.00110 0.00046 0.00010 -0.00017

41 4YY 0.00127 -0.00106 0.00028 -0.00013 -0.00113

42 4ZZ -0.00154 -0.00012 -0.00020 0.00056 0.00120

43 4XY -0.00157 0.00060 -0.00049 0.00038 0.00090

44 4XZ -0.00005 -0.00545 -0.00009 0.00041 0.00121

45 4YZ 0.01196 -0.00818 0.00167 -0.00309 -0.00746

46 4 C 1S 0.00180 -0.00010 0.00016 0.00033 0.00110

47 2S -0.00297 -0.00001 0.00024 -0.00067 -0.00165

48 2PX -0.03874 0.00013 -0.00413 0.00493 0.01537

49 2PY 0.01038 0.00064 0.00211 -0.00619 -0.01552

50 2PZ 0.24850 0.00092 0.03600 -0.06161 -0.15278

51 3S -0.02167 0.00311 -0.00582 -0.00473 -0.01272

52 3PX -0.02128 -0.00166 0.02712 0.00851 0.01554

53 3PY -0.00121 -0.00022 0.01020 0.01084 -0.01937

54 3PZ 0.17263 -0.00165 0.02886 -0.04212 -0.10528

55 4XX 0.00035 -0.00322 0.00007 -0.00027 -0.00134

56 4YY -0.00043 -0.00140 -0.00028 0.00026 0.00125

57 4ZZ 0.00031 0.00463 0.00003 0.00010 0.00028

58 4XY -0.00012 0.00247 0.00031 -0.00005 -0.00080

59 4XZ 0.00046 0.01515 -0.00044 0.00244 0.00639

60 4YZ -0.00022 -0.01133 -0.00073 0.00344 0.00924

61 5 C 1S -0.00018 -0.00006 0.00114 -0.00078 0.00031

62 2S 0.00029 0.00029 -0.00357 0.00120 -0.00075

63 2PX -0.00484 0.03506 -0.00184 0.00796 0.01739

64 2PY 0.00414 -0.02083 -0.00565 -0.00131 -0.01166

65 2PZ 0.09467 -0.29260 0.02014 -0.05218 -0.13216

66 3S 0.00311 -0.00162 0.01309 0.01062 0.00126

67 3PX 0.00369 0.02285 0.01825 0.00299 0.01901

68 3PY 0.00423 -0.01397 -0.01061 -0.00778 -0.00700

69 3PZ 0.06574 -0.20624 0.01621 -0.03726 -0.09417

70 4XX -0.00225 -0.00133 -0.00004 0.00055 0.00147

71 4YY 0.00026 0.00104 -0.00002 0.00003 0.00004

72 4ZZ 0.00197 0.00027 0.00021 -0.00066 -0.00141

73 4XY 0.00032 -0.00052 0.00055 -0.00060 -0.00044

74 4XZ 0.01152 0.00623 0.00160 -0.00258 -0.00655

75 4YZ 0.00368 0.00824 0.00033 0.00000 0.00017

76 6 C 1S 0.00024 -0.00002 -0.00064 0.00045 -0.00007

77 2S -0.00068 -0.00004 0.00157 -0.00065 0.00012

78 2PX 0.01354 0.03522 0.00315 -0.00347 -0.00586

79 2PY -0.01015 -0.02146 0.00244 -0.00044 0.00372

80 2PZ -0.13369 -0.29363 -0.01526 0.01821 0.04734

81 3S 0.00213 0.00075 -0.00131 -0.00941 0.00261

82 3PX 0.00958 0.02581 -0.00458 -0.00540 -0.00424

83 3PY -0.00434 -0.01576 0.00641 -0.00212 0.00470

84 3PZ -0.09399 -0.20803 -0.01149 0.01154 0.03026

85 4XX 0.00062 0.00116 0.00003 0.00013 0.00033

86 4YY 0.00110 -0.00109 -0.00003 -0.00053 -0.00139

87 4ZZ -0.00160 -0.00008 -0.00024 0.00048 0.00105

88 4XY -0.00129 0.00062 -0.00011 0.00041 0.00118

89 4XZ -0.00105 -0.00564 0.00003 -0.00043 -0.00114

90 4YZ 0.01065 -0.00873 0.00177 -0.00398 -0.01014

91 7 C 1S 0.00234 -0.00043 0.00605 -0.00280 0.00028

92 2S -0.00705 0.00150 -0.01478 0.00706 -0.00136

93 2PX 0.00704 -0.00027 0.00438 -0.00312 -0.02225

94 2PY -0.00498 0.00163 -0.02283 0.01104 0.01446

95 2PZ 0.04613 -0.00455 -0.00947 0.07504 0.20258

96 3S 0.00131 -0.00055 -0.01918 -0.00075 0.00906

97 3PX -0.01074 0.00032 -0.00687 0.00852 -0.02786

98 3PY -0.00744 -0.00066 0.02641 0.00466 0.01177

99 3PZ 0.02465 -0.00039 -0.01155 0.04892 0.13292

100 4XX 0.00367 -0.00040 0.00423 -0.00123 0.00103

101 4YY -0.00275 0.00001 -0.00176 0.00110 0.00137

102 4ZZ -0.00034 0.00027 0.00064 -0.00105 -0.00229

103 4XY -0.00190 0.00041 -0.00088 -0.00110 -0.00329

104 4XZ -0.00870 0.00091 0.00049 -0.00034 0.00023

105 4YZ -0.01294 -0.00053 -0.00287 0.00573 0.01414

106 8 N 1S -0.00710 0.00104 -0.00913 0.00160 -0.00106

107 2S 0.01437 -0.00243 0.01941 -0.00351 0.00191

108 2PX -0.02874 0.00330 -0.07036 0.01400 -0.05294

109 2PY 0.00304 -0.00187 0.02203 0.00445 0.02008

110 2PZ -0.09260 0.00930 -0.04710 0.08673 0.19986

111 3S 0.03374 -0.00325 0.02034 -0.00205 -0.00010

112 3PX -0.01678 0.00290 -0.05239 0.01030 -0.03851

113 3PY 0.00156 -0.00227 0.02180 -0.00108 0.01884

114 3PZ -0.06816 0.00103 -0.03475 0.06395 0.14228

115 4XX -0.00023 -0.00018 -0.00237 0.00033 -0.00143

116 4YY -0.00164 0.00035 -0.00166 -0.00072 -0.00299

117 4ZZ -0.00095 0.00003 0.00081 0.00083 0.00391

118 4XY 0.00007 -0.00010 0.00174 0.00025 0.00287

119 4XZ -0.00821 0.00134 -0.00233 0.00154 0.00168

120 4YZ -0.00132 0.00070 0.00186 -0.00636 -0.01639

121 9 N 1S 0.00126 -0.00074 0.00092 0.00144 -0.00420

122 2S -0.00272 0.00147 -0.00533 -0.00140 0.00845

123 2PX 0.03494 -0.00493 0.03714 -0.00393 0.04742

124 2PY -0.01816 0.00553 -0.01745 -0.00239 -0.02253

125 2PZ -0.09188 0.02042 0.00863 -0.08103 -0.22087

126 3S -0.00466 0.00375 0.02510 -0.02214 0.03082

127 3PX 0.01948 -0.00320 0.02586 -0.00745 0.03446

128 3PY -0.01236 0.00384 -0.01777 -0.00014 -0.01751

129 3PZ -0.07300 0.01766 0.00587 -0.06327 -0.15811

130 4XX -0.00041 -0.00013 -0.00075 0.00185 0.00186

131 4YY 0.00046 -0.00036 0.00005 0.00039 0.00093

132 4ZZ -0.00013 0.00019 -0.00046 -0.00143 -0.00482

133 4XY -0.00251 0.00039 -0.00384 0.00049 -0.00432

134 4XZ 0.00427 -0.00029 0.00254 -0.00544 -0.01226

135 4YZ 0.00710 -0.00138 -0.00042 0.00405 0.01001

136 10 C 1S -0.00728 0.00072 0.01173 -0.01155 0.00249

137 2S 0.01678 -0.00191 -0.02243 0.02428 -0.00465

138 2PX -0.00344 0.00080 -0.09201 0.06492 0.00359

139 2PY 0.01121 -0.00161 0.00212 -0.00449 -0.02268

140 2PZ 0.03083 0.00166 0.01515 -0.07108 -0.19051

141 3S 0.03591 -0.00243 -0.08530 0.08137 -0.02470

142 3PX -0.00330 0.00053 -0.03500 0.04363 -0.00169

143 3PY -0.00786 -0.00049 -0.03621 0.03088 -0.04382

144 3PZ 0.02435 -0.00178 0.01485 -0.03709 -0.13112

145 4XX -0.00294 0.00020 -0.00311 0.00116 -0.00355

146 4YY -0.00281 0.00059 0.00263 -0.00358 -0.00233

147 4ZZ 0.00433 -0.00056 0.00016 0.00168 0.00565

148 4XY -0.00372 -0.00001 -0.00032 -0.00021 -0.00219

149 4XZ 0.01755 -0.00115 0.00027 0.00573 0.01594

150 4YZ 0.00372 0.00129 0.00041 -0.00239 -0.00637

151 11 O 1S 0.00331 -0.00003 0.00057 0.00184 0.00291

152 2S -0.00612 -0.00005 -0.00027 -0.00639 -0.00479

153 2PX -0.01132 0.00392 -0.02168 -0.00163 -0.01415

154 2PY -0.02513 0.00039 0.02897 -0.01589 -0.00569

155 2PZ -0.10421 -0.01543 -0.00493 -0.00368 -0.00524

156 3S -0.02339 0.00070 -0.00343 -0.00163 -0.02583

157 3PX -0.00909 0.00200 -0.01553 0.00337 -0.01307

158 3PY -0.02114 0.00048 0.00869 -0.00431 -0.01037

159 3PZ -0.08169 -0.00768 -0.00513 -0.00295 -0.00499

160 4XX 0.00120 -0.00006 -0.00053 0.00139 0.00339

161 4YY -0.00023 -0.00018 0.00091 -0.00075 -0.00049

162 4ZZ 0.00217 0.00009 -0.00050 -0.00093 0.00004

163 4XY 0.00142 0.00006 -0.00327 0.00186 -0.00053

164 4XZ 0.00253 0.00000 0.00043 -0.00233 -0.00729

165 4YZ -0.00464 -0.00107 0.00021 -0.00200 -0.00477

166 12 S 1S -0.00143 0.00005 0.00485 -0.00307 0.00258

167 2S 0.00692 -0.00021 -0.02301 0.01501 -0.01359

168 2PX 0.01729 -0.00075 -0.00998 0.00824 0.00923

169 2PY 0.04926 -0.00257 -0.01900 0.02102 0.02519

170 2PZ -0.16170 0.00841 -0.02048 -0.03221 -0.14606

171 3S -0.01423 0.00070 0.05009 -0.03042 0.02271

172 3PX -0.04627 0.00198 0.02891 -0.02473 -0.02478

173 3PY -0.13106 0.00690 0.04983 -0.05645 -0.06769

174 3PZ 0.43042 -0.02246 0.05485 0.08700 0.39432

175 4S -0.01821 -0.00088 0.06564 -0.05522 0.07314

176 4PX -0.02072 0.00007 -0.02282 0.04134 -0.02773

177 4PY -0.06711 0.00498 0.03852 -0.03632 -0.05905

178 4PZ 0.23505 -0.01134 0.02710 0.05164 0.22172

179 5XX 0.00765 -0.00034 -0.02691 0.01938 -0.01301

180 5YY 0.00145 -0.00003 0.01516 -0.01072 0.00483

181 5ZZ -0.00749 0.00031 0.00733 -0.00562 0.00449

182 5XY 0.00047 -0.00003 0.00647 -0.00144 0.00777

183 5XZ -0.01015 0.00025 -0.00750 0.00489 0.01048

184 5YZ -0.00894 0.00060 0.00441 -0.00641 -0.00332

185 13 C 1S -0.00316 0.00010 -0.00017 0.00083 0.00260

186 2S 0.00612 -0.00060 0.00291 -0.00397 -0.00392

187 2PX 0.04055 -0.00249 -0.21361 0.14536 -0.03553

188 2PY 0.03518 -0.00167 -0.11413 0.06828 -0.04305

189 2PZ -0.02743 0.00120 -0.09443 0.04863 -0.05963

190 3S 0.02578 0.00017 -0.00976 0.01407 -0.00945

191 3PX 0.02463 -0.00228 -0.16325 0.10108 -0.02897

192 3PY 0.00084 0.00183 -0.07088 0.02142 -0.06587

193 3PZ 0.02964 -0.00208 -0.05637 0.05472 0.01360

194 4XX 0.00028 -0.00005 0.00140 0.00346 -0.00035

195 4YY -0.00597 0.00018 0.00481 0.00264 -0.00735

196 4ZZ 0.00543 -0.00030 -0.00569 -0.00657 0.00779

197 4XY 0.00126 -0.00013 0.00569 0.00704 0.00011

198 4XZ -0.00542 0.00038 -0.00963 -0.01085 -0.00224

199 4YZ 0.00900 -0.00043 -0.00187 -0.00149 0.00852

200 14 C 1S -0.01432 0.00075 -0.00148 -0.00376 -0.01386

201 2S 0.03071 -0.00167 0.00208 0.00804 0.02879

202 2PX -0.04225 0.00124 0.06888 0.19893 -0.10220

203 2PY 0.02725 -0.00200 0.03846 0.11456 -0.00880

204 2PZ 0.03321 -0.00219 0.03590 0.09785 0.00436

205 3S 0.08912 -0.00494 0.01928 0.02611 0.10538

206 3PX -0.01683 0.00014 0.04564 0.15646 -0.06817

207 3PY 0.00406 -0.00085 0.02654 0.08617 -0.02725

208 3PZ 0.00634 -0.00052 0.03587 0.06660 -0.01286

209 4XX -0.00358 0.00016 0.01449 -0.00426 0.00080

210 4YY -0.00154 0.00007 -0.00796 0.00046 -0.00326

211 4ZZ 0.00223 -0.00012 -0.00713 0.00326 0.00002

212 4XY 0.00258 -0.00012 -0.00391 0.00059 0.00171

213 4XZ 0.00045 -0.00003 -0.00633 0.00303 -0.00128

214 4YZ -0.00004 0.00001 -0.00901 0.00213 -0.00359

215 15 C 1S 0.00615 -0.00035 0.00048 0.00193 0.00687

216 2S -0.01315 0.00071 -0.00138 -0.00368 -0.01392

217 2PX -0.02196 0.00048 0.26956 0.01208 0.03005

218 2PY -0.04559 0.00213 0.13459 -0.00343 -0.01876

219 2PZ -0.02848 0.00121 0.11321 0.00038 -0.00442

220 3S -0.02990 0.00173 -0.00236 -0.01028 -0.04278

221 3PX -0.01618 0.00052 0.20617 0.00386 0.03087

222 3PY -0.04027 0.00193 0.10584 -0.00777 -0.02258

223 3PZ -0.01408 0.00055 0.08425 -0.00019 0.00203

224 4XX 0.00077 -0.00001 -0.00085 -0.00720 0.00339

225 4YY 0.00040 -0.00005 -0.00207 0.01053 -0.00410

226 4ZZ 0.00072 -0.00004 0.00301 -0.00271 0.00264

227 4XY 0.00063 -0.00007 -0.00269 0.00986 -0.00358

228 4XZ -0.00150 0.00009 0.00360 -0.00625 0.00169

229 4YZ 0.00022 -0.00002 0.00113 0.00311 -0.00053

230 16 C 1S -0.00139 0.00005 -0.00010 -0.00062 -0.00094

231 2S 0.00336 -0.00019 -0.00016 0.00208 0.00240

232 2PX -0.02794 0.00175 0.13847 -0.19879 0.07884

233 2PY -0.01138 0.00076 0.07007 -0.10030 0.04109

234 2PZ -0.01024 0.00074 0.06071 -0.08408 0.03430

235 3S 0.00337 0.00067 0.00619 -0.00551 -0.00149

236 3PX -0.01399 0.00059 0.07798 -0.13460 0.05569

237 3PY -0.01637 0.00106 0.04047 -0.07124 0.02009

238 3PZ 0.00075 0.00057 0.03412 -0.05905 0.02783

239 4XX 0.00160 -0.00012 -0.00499 0.01397 -0.00512

240 4YY -0.00334 0.00016 0.01095 -0.00671 0.00171

241 4ZZ 0.00136 -0.00002 -0.00606 -0.00739 0.00302

242 4XY -0.00112 0.00004 0.01139 -0.00303 0.00253

243 4XZ 0.00061 -0.00001 -0.00975 -0.00676 0.00145

244 4YZ -0.00072 0.00006 0.00116 -0.00842 0.00281

245 17 C 1S -0.00436 0.00022 -0.00035 -0.00112 -0.00213

246 2S 0.00857 -0.00039 0.00066 0.00210 0.00341

247 2PX -0.01172 0.00155 -0.06183 -0.23660 0.07396

248 2PY 0.00687 0.00011 -0.03258 -0.11646 0.04084

249 2PZ -0.00155 0.00040 -0.02733 -0.09918 0.03177

250 3S 0.03125 -0.00277 -0.00298 0.00940 0.02481

251 3PX -0.01606 0.00156 -0.03560 -0.15065 0.03969

252 3PY 0.01460 -0.00068 -0.01826 -0.06882 0.03752

253 3PZ 0.00655 0.00075 -0.01244 -0.07064 0.02131

254 4XX -0.00069 -0.00003 0.01269 0.00093 0.00114

255 4YY -0.00142 0.00014 -0.00969 -0.01155 0.00210

256 4ZZ 0.00107 -0.00010 -0.00336 0.01029 -0.00360

257 4XY -0.00024 0.00011 -0.00713 -0.01240 0.00352

258 4XZ -0.00004 -0.00004 -0.00173 0.01344 -0.00558

259 4YZ 0.00267 -0.00010 -0.00660 0.00192 -0.00001

260 18 C 1S 0.01148 -0.00063 0.00120 0.00318 0.00900

261 2S -0.02317 0.00137 -0.00242 -0.00474 -0.01722

262 2PX 0.02284 0.00023 -0.25084 -0.13203 0.02947

263 2PY -0.03658 0.00262 -0.12716 -0.07485 -0.01655

264 2PZ 0.03681 -0.00075 -0.10058 -0.04869 0.03004

265 3S -0.09429 0.00598 -0.00373 -0.04423 -0.09714

266 3PX 0.00602 0.00045 -0.16953 -0.10862 0.02159

267 3PY -0.01279 0.00070 -0.08759 -0.07239 -0.00575

268 3PZ 0.02752 -0.00211 -0.07924 -0.02103 0.03747

269 4XX 0.00055 0.00006 -0.00357 -0.01068 0.00402

270 4YY 0.00235 -0.00010 -0.00313 0.01010 -0.00290

271 4ZZ -0.00049 0.00003 0.00709 0.00133 0.00065

272 4XY 0.00081 -0.00007 -0.00489 0.00809 -0.00249

273 4XZ -0.00085 0.00002 0.00832 -0.00109 0.00065

274 4YZ -0.00016 -0.00002 0.00289 0.00558 -0.00180

275 19 C 1S 0.00553 0.00014 -0.00009 0.00130 0.00452

276 2S -0.01101 0.00121 -0.00001 -0.00112 -0.00994

277 2PX 0.00421 0.00077 0.07733 0.03074 0.00296

278 2PY -0.05114 0.00353 0.03364 0.00647 -0.04219

279 2PZ -0.01330 0.00054 0.02895 0.00849 -0.01232

280 3S -0.02844 -0.00700 0.00462 -0.01863 -0.02322

281 3PX 0.00896 0.00533 0.03293 0.01873 0.00267

282 3PY -0.03290 0.00521 0.01756 0.01101 -0.03604

283 3PZ -0.01811 0.00067 0.00687 0.00206 -0.01832

284 4XX 0.00158 0.00007 -0.00945 -0.00524 0.00165

285 4YY -0.00117 0.00030 0.00127 0.00146 -0.00127

286 4ZZ -0.00073 0.00030 0.00799 0.00389 -0.00105

287 4XY 0.00031 -0.00010 -0.00789 -0.00307 0.00048

288 4XZ 0.00003 -0.00008 0.00864 0.00412 0.00005

289 4YZ -0.00172 0.00008 0.00311 0.00166 -0.00203

290 20 O 1S 0.00336 -0.00018 0.00149 0.00192 0.00189

291 2S -0.00767 0.00039 -0.00363 -0.00454 -0.00465

292 2PX 0.01310 -0.00205 0.08724 0.24387 -0.07296

293 2PY -0.00806 -0.00040 0.04248 0.12402 -0.04571

294 2PZ 0.00638 -0.00088 0.03396 0.10739 -0.03185

295 3S -0.01817 0.00083 -0.00696 -0.00796 -0.00882

296 3PX 0.01063 -0.00179 0.06949 0.20702 -0.06232

297 3PY -0.00520 -0.00040 0.03453 0.10751 -0.03863

298 3PZ 0.00503 -0.00071 0.02700 0.09139 -0.02785

299 4XX 0.00089 -0.00012 0.00362 0.01005 -0.00276

300 4YY 0.00061 -0.00003 -0.00158 -0.00464 0.00179

301 4ZZ -0.00004 0.00003 -0.00168 -0.00467 0.00155

302 4XY -0.00063 0.00004 -0.00081 -0.00278 0.00056

303 4XZ -0.00050 0.00007 -0.00195 -0.00356 0.00075

304 4YZ 0.00038 0.00001 -0.00195 -0.00540 0.00207

305 21 O 1S 0.00103 -0.00005 0.00015 0.00066 0.00089

306 2S -0.00210 0.00010 -0.00029 -0.00133 -0.00203

307 2PX 0.03553 -0.00202 -0.15446 0.16919 -0.06500

308 2PY 0.00926 -0.00059 -0.07903 0.08417 -0.04095

309 2PZ 0.01708 -0.00099 -0.06896 0.07512 -0.02709

310 3S -0.00925 0.00051 -0.00165 -0.00440 -0.00783

311 3PX 0.02926 -0.00169 -0.12420 0.15043 -0.05751

312 3PY 0.00740 -0.00046 -0.06346 0.07512 -0.03587

313 3PZ 0.01364 -0.00087 -0.05501 0.06676 -0.02359

314 4XX 0.00075 -0.00005 -0.00305 0.00503 -0.00182

315 4YY 0.00037 -0.00002 -0.00049 0.00023 0.00011

316 4ZZ -0.00053 0.00003 0.00364 -0.00473 0.00201

317 4XY 0.00050 -0.00003 -0.00152 0.00155 -0.00055

318 4XZ -0.00089 0.00005 0.00377 -0.00522 0.00200

319 4YZ -0.00032 0.00002 0.00198 -0.00308 0.00132

320 22 H 1S -0.00009 -0.00016 0.00087 -0.00018 0.00011

321 2S -0.00016 -0.00041 0.00243 0.00076 0.00011

322 23 H 1S 0.00025 -0.00003 -0.00045 -0.00005 0.00057

323 2S 0.00070 0.00034 -0.00290 -0.00288 0.00145

324 24 H 1S 0.00076 0.00005 0.00124 -0.00037 0.00038

325 2S 0.00157 -0.00132 0.01466 0.01521 -0.00159

326 25 H 1S -0.00182 0.00015 -0.00389 0.00152 -0.00088

327 2S 0.00384 -0.00107 0.00998 0.00024 0.00331

328 26 H 1S 0.00205 -0.00004 0.00011 0.00035 0.00048

329 2S 0.00202 0.00025 -0.00248 0.00024 0.00012

330 27 H 1S 0.00945 -0.00059 0.00004 0.00298 0.01156

331 2S -0.00973 0.00075 0.00369 -0.00592 -0.00470

332 28 H 1S 0.01063 -0.00057 0.00102 0.00278 0.00974

333 2S 0.01810 -0.00100 0.00153 0.00509 0.01867

334 29 H 1S -0.02409 0.00163 0.02920 0.01123 -0.01904

335 2S -0.00196 -0.00001 0.03831 0.01945 0.00526

336 30 H 1S 0.00585 -0.00032 0.05167 0.02362 0.00367

337 2S 0.00786 -0.00065 0.07054 0.04269 0.00250

338 31 H 1S 0.01055 -0.00139 -0.08248 -0.03496 0.01046

339 2S 0.01700 0.01065 -0.10760 -0.04873 0.01043

340 32 H 1S 0.00693 -0.00035 0.00290 0.00459 0.00294

341 2S 0.01103 -0.00056 0.00300 0.00791 0.00640

342 33 H 1S 0.00041 -0.00002 -0.00011 0.00121 0.00002

343 2S 0.00367 -0.00015 0.00133 0.00231 0.00390

79 80 81 82 83

V V V V V

Eigenvalues -- -0.04615 -0.02057 -0.00931 -0.00613 0.01342

1 1 C 1S -0.00009 -0.00012 -0.00020 -0.00021 -0.00141

2 2S 0.00021 -0.00022 0.00040 0.00047 0.00298

3 2PX -0.03261 -0.00173 0.00392 0.00358 0.01369

4 2PY 0.01998 0.00128 -0.00234 -0.00224 -0.00800

5 2PZ 0.27227 0.01179 -0.02939 -0.02374 -0.11435

6 3S 0.00063 0.00670 0.00182 -0.00011 0.01420

7 3PX -0.03824 0.00440 0.00403 0.00253 0.01749

8 3PY 0.02359 0.00280 -0.00309 -0.00331 -0.01286

9 3PZ 0.32213 0.01516 -0.04002 -0.03197 -0.16081

10 4XX 0.00070 0.00018 -0.00478 0.00146 0.00014

11 4YY -0.00064 -0.00039 -0.00191 0.00088 0.00066

12 4ZZ -0.00007 0.00017 0.00665 -0.00245 -0.00095

13 4XY 0.00035 0.00015 0.00341 -0.00149 -0.00113

14 4XZ -0.00349 0.00067 0.02213 -0.00764 -0.00129

15 4YZ -0.00525 -0.00086 -0.01531 0.00649 0.00565

16 2 C 1S 0.00023 -0.00054 0.00010 0.00013 -0.00021

17 2S -0.00035 0.00169 -0.00038 -0.00101 0.00115

18 2PX 0.01020 -0.00034 -0.03678 0.01101 -0.00225

19 2PY -0.00712 0.00173 0.02114 -0.00833 0.00017

20 2PZ -0.08893 0.00582 0.30571 -0.09496 0.02397

21 3S -0.00355 -0.00375 0.00039 0.00112 -0.00243

22 3PX 0.01298 0.00938 -0.05047 0.01132 -0.00481

23 3PY -0.01016 -0.00500 0.02958 -0.00747 -0.00421

24 3PZ -0.11319 0.01119 0.40764 -0.12510 0.03821

25 4XX 0.00404 0.00022 0.00154 -0.00091 -0.00164

26 4YY -0.00086 -0.00039 -0.00163 0.00057 -0.00010

27 4ZZ -0.00317 -0.00013 0.00010 0.00029 0.00171

28 4XY -0.00062 -0.00009 0.00111 -0.00011 0.00053

29 4XZ -0.01942 -0.00113 -0.00696 0.00517 0.00960

30 4YZ -0.00710 -0.00059 -0.01260 0.00549 0.00371

31 3 C 1S -0.00067 0.00169 -0.00092 -0.00125 -0.00238

32 2S 0.00152 -0.00362 0.00249 0.00307 0.00587

33 2PX 0.02430 0.00261 0.03553 -0.00997 -0.00440

34 2PY -0.01249 -0.00517 -0.01928 0.00878 0.00839

35 2PZ -0.19858 -0.01569 -0.27200 0.12184 0.09233

36 3S 0.00884 -0.00073 0.00345 0.00458 0.02623

37 3PX 0.02671 -0.01631 0.05221 -0.00906 -0.00099

38 3PY -0.01643 0.00825 -0.03200 0.00311 -0.00161

39 3PZ -0.23265 -0.03014 -0.37113 0.15595 0.10904

40 4XX 0.00022 0.00058 0.00216 -0.00070 -0.00156

41 4YY 0.00193 0.00060 -0.00199 0.00017 -0.00027

42 4ZZ -0.00208 -0.00015 -0.00013 0.00043 0.00165

43 4XY -0.00197 0.00008 0.00098 -0.00036 0.00122

44 4XZ -0.00079 -0.00054 -0.01016 0.00386 0.00214

45 4YZ 0.01510 0.00031 -0.01547 0.00304 -0.00757

46 4 C 1S -0.00047 0.00137 -0.00073 -0.00072 -0.00634

47 2S 0.00085 -0.00379 0.00207 0.00077 0.01529

48 2PX -0.02728 -0.00728 0.00476 0.00535 0.03092

49 2PY 0.01848 -0.00454 0.00126 0.00049 0.01227

50 2PZ 0.24128 0.01425 -0.02187 -0.02777 -0.12606

51 3S 0.00511 -0.00517 0.00786 0.02588 0.04433

52 3PX -0.03814 -0.01071 0.01151 0.02432 0.01157

53 3PY 0.02510 0.02129 -0.00511 0.00291 0.00169

54 3PZ 0.28362 0.01770 -0.02122 -0.02835 -0.15365

55 4XX -0.00343 0.00183 0.00466 -0.00182 -0.00253

56 4YY 0.00275 -0.00114 0.00222 -0.00072 0.00088

57 4ZZ 0.00055 -0.00027 -0.00694 0.00244 0.00104

58 4XY -0.00153 0.00082 -0.00396 0.00127 -0.00130

59 4XZ 0.01354 -0.00030 -0.02336 0.00795 0.00310

60 4YZ 0.01855 0.00122 0.01590 -0.00662 -0.00145

61 5 C 1S 0.00058 -0.00289 0.00051 0.00056 0.00139

62 2S -0.00130 0.00604 -0.00133 -0.00160 -0.00215

63 2PX 0.02066 0.00540 -0.03746 0.01106 -0.00930

64 2PY -0.01392 0.00422 0.02133 -0.00834 0.00366

65 2PZ -0.19453 0.00369 0.30029 -0.09641 -0.01573

66 3S -0.00729 0.02356 -0.00065 0.00108 -0.02175

67 3PX 0.02358 -0.01339 -0.04240 0.02381 -0.01641

68 3PY -0.01428 -0.00657 0.02984 -0.01223 0.01825

69 3PZ -0.22837 0.00279 0.39697 -0.12427 -0.00374

70 4XX -0.00306 -0.00064 -0.00158 0.00121 0.00288

71 4YY 0.00051 -0.00004 0.00156 -0.00069 -0.00102

72 4ZZ 0.00254 0.00013 0.00008 -0.00054 -0.00163

73 4XY 0.00071 -0.00123 -0.00063 0.00058 0.00109

74 4XZ 0.01441 0.00129 0.00834 -0.00548 -0.01031

75 4YZ 0.00417 0.00055 0.01308 -0.00521 -0.00318

76 6 C 1S -0.00032 0.00158 -0.00048 -0.00056 -0.00205

77 2S 0.00058 -0.00311 0.00096 0.00093 0.00435

78 2PX 0.01185 -0.00101 0.03404 -0.01362 -0.01251

79 2PY -0.00613 -0.00547 -0.01933 0.00975 0.01243

80 2PZ -0.09431 -0.01695 -0.27843 0.11993 0.11262

81 3S 0.00327 -0.02354 0.00564 0.00575 0.02281

82 3PX 0.01533 -0.00153 0.04353 -0.01847 -0.01793

83 3PY -0.00760 -0.01453 -0.02287 0.01518 0.02053

84 3PZ -0.11793 -0.02073 -0.36674 0.15774 0.14686

85 4XX 0.00000 0.00021 -0.00215 0.00069 -0.00033

86 4YY -0.00251 -0.00010 0.00189 -0.00041 0.00134

87 4ZZ 0.00245 0.00020 0.00013 -0.00046 -0.00135

88 4XY 0.00239 0.00020 -0.00110 0.00005 -0.00112

89 4XZ -0.00078 0.00042 0.00958 -0.00384 -0.00336

90 4YZ -0.02048 -0.00041 0.01474 -0.00311 0.00522

91 7 C 1S 0.00084 -0.00611 0.00117 0.00081 0.00817

92 2S -0.00153 0.01386 -0.00296 -0.00042 -0.01552

93 2PX -0.03980 0.02200 -0.00283 0.00238 -0.03973

94 2PY 0.02248 0.00056 -0.00031 -0.00199 0.01419

95 2PZ 0.25011 0.00524 0.00100 0.00681 0.08237

96 3S -0.00853 0.02345 0.00414 0.00339 -0.07647

97 3PX -0.03097 0.05304 -0.00777 0.00138 -0.03732

98 3PY 0.01737 -0.01381 0.01630 0.04340 -0.00738

99 3PZ 0.21534 0.00346 -0.01117 -0.00226 0.07652

100 4XX 0.00254 -0.00305 0.00203 0.00195 0.00338

101 4YY -0.00312 0.00096 0.00093 0.00063 0.00358

102 4ZZ 0.00110 0.00005 -0.00195 -0.00040 -0.00440

103 4XY 0.00290 -0.00222 -0.00025 0.00080 0.00287

104 4XZ -0.00991 -0.00124 -0.00447 0.00061 -0.00657

105 4YZ -0.02306 -0.00111 0.00551 0.00276 0.01595

106 8 N 1S -0.00025 -0.00453 0.00035 0.00133 -0.00434

107 2S 0.00047 0.01023 0.00032 -0.00216 0.00828

108 2PX 0.03671 0.04248 -0.00792 -0.01978 0.01720

109 2PY -0.02438 0.00751 0.00427 0.00490 0.03041

110 2PZ -0.26080 -0.00092 0.02153 0.03292 0.11745

111 3S 0.00454 0.04867 -0.01624 -0.03784 0.06202

112 3PX 0.03681 0.04400 -0.01111 -0.02542 0.03385

113 3PY -0.02620 -0.00387 0.01444 0.01651 0.01912

114 3PZ -0.25704 0.00467 0.04442 0.02533 0.11832

115 4XX 0.00224 -0.00167 0.00129 0.00067 0.00257

116 4YY -0.00099 0.00028 -0.00096 -0.00094 -0.00391

117 4ZZ -0.00126 -0.00050 0.00046 0.00076 0.00024

118 4XY 0.00007 -0.00136 0.00054 0.00069 0.00161

119 4XZ -0.00861 0.00005 -0.00262 0.00018 -0.00552

120 4YZ -0.00591 -0.00022 -0.00428 -0.00208 -0.01797

121 9 N 1S 0.00111 0.01122 -0.00099 -0.00436 0.01239

122 2S -0.00290 -0.01827 -0.00059 0.00057 -0.02151

123 2PX -0.00317 -0.02320 0.01466 0.01687 0.02997

124 2PY -0.00384 0.02754 -0.01461 -0.01491 -0.04503

125 2PZ 0.00056 -0.00192 -0.08188 -0.04847 -0.33759

126 3S -0.00262 -0.14288 0.02989 0.10478 -0.14952

127 3PX 0.00219 -0.04698 0.02857 0.04403 0.04037

128 3PY -0.00557 0.03888 -0.02275 -0.03850 -0.02011

129 3PZ -0.01154 -0.01785 -0.09749 -0.05059 -0.37166

130 4XX -0.00383 0.00580 -0.00115 -0.00251 0.00338

131 4YY 0.00072 -0.00224 0.00073 0.00007 0.00375

132 4ZZ 0.00352 0.00252 -0.00110 -0.00335 0.00089

133 4XY 0.00197 0.00223 -0.00053 -0.00170 0.00318

134 4XZ 0.01770 0.00017 0.00185 -0.00061 0.00743

135 4YZ 0.00078 0.00087 0.00174 0.00059 0.00358

136 10 C 1S 0.00438 -0.04656 0.01009 0.01656 0.02165

137 2S -0.00908 0.09150 -0.01869 -0.03120 -0.03915

138 2PX -0.03883 0.15491 -0.03935 -0.05664 -0.08219

139 2PY 0.02245 0.01967 0.01053 -0.00134 0.07574

140 2PZ 0.18987 0.02635 0.07278 0.01760 0.32644

141 3S -0.03257 0.44852 -0.10520 -0.17904 -0.20805

142 3PX -0.02597 0.14907 -0.02698 -0.00031 -0.14871

143 3PY 0.02000 0.14375 -0.00990 -0.06439 0.15127

144 3PZ 0.17552 0.04128 0.10227 0.06585 0.35779

145 4XX -0.00117 -0.00312 -0.00069 0.00060 -0.00826

146 4YY 0.00381 -0.00685 0.00153 0.00246 0.00952

147 4ZZ -0.00147 0.00003 0.00153 0.00070 0.00530

148 4XY 0.00145 0.00011 0.00267 0.00187 0.01813

149 4XZ 0.00233 0.00019 0.00413 0.00378 0.01849

150 4YZ 0.01084 -0.00020 -0.00317 -0.00091 -0.00468

151 11 O 1S -0.00255 0.00590 -0.00255 -0.00021 -0.01865

152 2S 0.00564 -0.01688 0.00528 -0.00105 0.03553

153 2PX 0.03362 -0.00179 0.00484 -0.00069 0.05618

154 2PY -0.01050 -0.03104 0.00902 0.01629 0.03036

155 2PZ -0.19684 -0.00767 -0.01554 -0.02565 -0.17219

156 3S 0.01950 -0.02530 0.02090 0.00275 0.18048

157 3PX 0.03209 0.01562 0.00866 0.00361 0.06031

158 3PY -0.00883 -0.01410 0.00636 0.00439 0.05586

159 3PZ -0.18970 -0.00763 -0.03397 -0.01973 -0.18384

160 4XX -0.00007 0.00081 -0.00135 -0.00003 -0.00982

161 4YY -0.00038 0.00000 0.00005 -0.00106 -0.00153

162 4ZZ -0.00128 -0.00053 -0.00078 -0.00163 -0.00400

163 4XY -0.00078 0.00657 -0.00203 -0.00355 -0.00371

164 4XZ -0.00400 0.00086 0.00334 0.00136 0.00713

165 4YZ -0.00152 0.00069 0.00420 -0.00073 0.00858

166 12 S 1S -0.00098 -0.00730 0.00043 0.00151 -0.00558

167 2S 0.00711 0.03520 -0.00093 -0.00531 0.03137

168 2PX 0.00898 -0.05587 0.01557 0.02418 0.06067

169 2PY -0.01263 0.01240 -0.00785 -0.00818 -0.05174

170 2PZ 0.02948 0.00800 0.00980 0.00320 0.03726

171 3S -0.00291 -0.07702 0.00803 0.02215 -0.04629

172 3PX -0.02436 0.15317 -0.04295 -0.06746 -0.16833

173 3PY 0.03492 -0.03160 0.02076 0.02021 0.14623

174 3PZ -0.08287 -0.02108 -0.02700 -0.00827 -0.10433

175 4S -0.07979 -0.18079 -0.01462 -0.01950 -0.22398

176 4PX -0.04756 0.34412 -0.07649 -0.10313 -0.33939

177 4PY 0.07699 -0.08264 0.05405 0.09375 0.26427

178 4PZ -0.05147 -0.01598 -0.03326 -0.01518 -0.08786

179 5XX 0.00530 0.07894 -0.00815 -0.02249 0.01259

180 5YY 0.00667 -0.05218 0.01237 0.02291 0.02865

181 5ZZ -0.00860 -0.02118 -0.00293 0.00031 -0.02950

182 5XY -0.01040 0.00225 -0.00628 -0.00019 -0.06946

183 5XZ -0.02665 0.01124 -0.01763 -0.01869 -0.06202

184 5YZ 0.00059 -0.01786 0.00001 0.00235 -0.00165

185 13 C 1S -0.00925 0.00896 -0.00661 -0.00688 -0.04504

186 2S 0.01391 -0.02296 0.01540 0.01511 0.08854

187 2PX -0.02778 0.26384 -0.04864 -0.09937 -0.02533

188 2PY 0.02880 0.08915 0.00654 -0.02170 0.19164

189 2PZ 0.00973 0.09600 -0.00718 -0.02927 0.07084

190 3S 0.07701 -0.05405 0.05008 0.06163 0.38034

191 3PX -0.03943 0.35394 -0.06996 -0.16511 -0.01302

192 3PY 0.07302 0.07185 0.01414 -0.01428 0.29617

193 3PZ -0.03077 0.08098 0.00521 0.00903 0.08872

194 4XX -0.00055 -0.01142 0.00399 0.01210 -0.00751

195 4YY 0.00119 0.01487 0.00172 0.00366 0.00065

196 4ZZ -0.00306 -0.00361 -0.00535 -0.01565 0.00113

197 4XY -0.00046 0.01500 0.00169 0.00712 -0.00005

198 4XZ 0.00041 -0.00454 -0.00615 -0.01972 0.00492

199 4YZ -0.00254 0.00443 -0.00447 -0.01023 -0.00340

200 14 C 1S 0.00435 0.00198 0.00080 -0.00129 0.00392

201 2S -0.00849 -0.00171 -0.00218 -0.00003 -0.00640

202 2PX 0.01971 -0.09667 0.09423 0.27835 -0.07008

203 2PY 0.00270 -0.05418 0.04800 0.14403 -0.02585

204 2PZ -0.00961 -0.04014 0.03355 0.11589 -0.07974

205 3S -0.05521 -0.05447 0.00637 0.04931 -0.01922

206 3PX 0.02325 -0.09464 0.12075 0.36776 -0.12390

207 3PY 0.01300 -0.05927 0.07505 0.20614 0.00340

208 3PZ -0.00065 -0.08429 0.06519 0.19454 -0.06867

209 4XX 0.00028 -0.01836 -0.00180 -0.00769 0.00093

210 4YY 0.00051 0.00866 0.00243 0.00758 -0.00132

211 4ZZ -0.00073 0.01042 -0.00055 -0.00046 0.00122

212 4XY -0.00061 0.00404 0.00147 0.00644 -0.00519

213 4XZ -0.00074 0.01061 -0.00175 -0.00338 -0.00148

214 4YZ 0.00173 0.01034 0.00217 0.00460 0.01018

215 15 C 1S -0.00373 0.00148 -0.00209 -0.00156 -0.01477

216 2S 0.00685 -0.00322 0.00444 0.00365 0.03047

217 2PX -0.01185 -0.16078 -0.07055 -0.22166 0.01220

218 2PY 0.00627 -0.08440 -0.03054 -0.11004 0.03806

219 2PZ -0.00177 -0.06873 -0.02969 -0.09471 -0.00229

220 3S 0.03326 0.00099 0.01954 0.00982 0.14682

221 3PX -0.01967 -0.21655 -0.10019 -0.31073 0.01959

222 3PY 0.01307 -0.12827 -0.03415 -0.14043 0.08195

223 3PZ -0.00570 -0.07134 -0.05026 -0.14736 -0.05014

224 4XX -0.00103 0.00616 -0.00543 -0.01578 0.00343

225 4YY 0.00105 -0.01341 0.00497 0.01398 -0.00370

226 4ZZ -0.00080 0.00786 -0.00001 0.00140 -0.00254

227 4XY 0.00052 -0.01301 0.00385 0.01064 -0.00498

228 4XZ 0.00025 0.01069 -0.00026 -0.00065 0.00548

229 4YZ -0.00030 -0.00139 0.00229 0.00786 -0.00493

230 16 C 1S -0.00046 0.00059 -0.00044 -0.00077 -0.00477

231 2S 0.00072 0.00086 0.00086 0.00105 0.00873

232 2PX -0.00830 0.28795 -0.02013 -0.03481 0.05665

233 2PY -0.00249 0.14607 -0.00939 -0.01825 0.03224

234 2PZ -0.00340 0.12457 -0.00914 -0.01639 0.02071

235 3S 0.01228 -0.03499 0.00932 0.01627 0.08768

236 3PX -0.00769 0.31619 -0.01654 -0.02676 0.06345

237 3PY -0.00113 0.13848 -0.00636 -0.00743 0.03971

238 3PZ -0.00282 0.13670 -0.01355 -0.02236 0.01805

239 4XX -0.00030 -0.00302 -0.00333 -0.01030 0.00220

240 4YY -0.00011 -0.00183 -0.00234 -0.00758 0.00032

241 4ZZ 0.00044 0.00499 0.00568 0.01782 -0.00264

242 4XY -0.00050 -0.00328 -0.00357 -0.01107 0.00340

243 4XZ 0.00070 0.00638 0.00683 0.02122 -0.00453

244 4YZ 0.00027 0.00280 0.00258 0.00802 -0.00264

245 17 C 1S -0.00089 0.00242 -0.00153 -0.00225 -0.01096

246 2S 0.00301 -0.00577 0.00442 0.00629 0.02652

247 2PX 0.00946 -0.01877 0.08987 0.27311 -0.09427

248 2PY 0.00779 -0.01568 0.04890 0.14083 -0.03079

249 2PZ 0.00606 -0.01310 0.04165 0.12174 -0.02009

250 3S -0.00176 0.00901 0.00290 -0.00820 0.06732

251 3PX 0.00908 -0.02135 0.10044 0.30787 -0.10727

252 3PY 0.00305 0.00433 0.05008 0.14027 -0.03165

253 3PZ 0.01261 -0.02652 0.04029 0.12441 -0.00075

254 4XX -0.00037 0.02431 0.00175 0.00753 0.00275

255 4YY 0.00000 -0.01038 -0.00086 -0.00344 -0.00390

256 4ZZ 0.00013 -0.01279 -0.00120 -0.00488 -0.00119

257 4XY 0.00036 -0.00628 0.00007 -0.00065 0.00058

258 4XZ -0.00003 -0.01199 -0.00147 -0.00493 -0.00238

259 4YZ 0.00055 -0.01515 -0.00040 -0.00335 0.00339

260 18 C 1S -0.00239 -0.00085 -0.00009 0.00097 -0.00149

261 2S 0.00213 0.00537 0.00083 -0.00099 0.00226

262 2PX 0.00142 -0.26325 -0.04798 -0.17233 0.00982

263 2PY 0.00433 -0.12553 -0.02520 -0.09044 0.00372

264 2PZ 0.00198 -0.11515 -0.01822 -0.06724 0.02766

265 3S 0.06256 -0.02480 0.00403 -0.00707 0.06108

266 3PX -0.00076 -0.32088 -0.04850 -0.17747 -0.01967

267 3PY 0.02100 -0.14233 -0.03333 -0.12999 0.02477

268 3PZ -0.01802 -0.10002 -0.02227 -0.08582 0.02054

269 4XX 0.00033 -0.00608 0.00486 0.01428 -0.00472

270 4YY 0.00004 0.00939 -0.00399 -0.01222 0.01145

271 4ZZ -0.00087 -0.00285 -0.00108 -0.00183 -0.00777

272 4XY -0.00135 0.01107 -0.00499 -0.01288 0.00112

273 4XZ 0.00038 -0.00835 0.00124 0.00287 0.00116

274 4YZ -0.00066 0.00142 -0.00242 -0.00699 0.00132

275 19 C 1S -0.00330 -0.00346 -0.00323 -0.00046 0.00081

276 2S 0.00465 0.00704 -0.00033 -0.00259 -0.00138

277 2PX -0.00986 0.01343 -0.00823 -0.00007 -0.01743

278 2PY 0.00876 0.00330 0.00207 0.00825 0.01806

279 2PZ 0.00535 0.00078 0.00505 0.00594 0.03322

280 3S 0.04556 0.01682 0.06033 0.02039 -0.00042

281 3PX -0.01719 -0.00518 -0.05606 -0.07088 -0.03057

282 3PY -0.00435 -0.03685 -0.00918 0.01202 0.01317

283 3PZ 0.02135 0.00794 -0.00135 -0.02972 0.07028

284 4XX 0.00003 -0.01325 -0.00241 -0.00715 -0.00006

285 4YY -0.00028 0.00299 -0.00119 -0.00094 0.00050

286 4ZZ -0.00026 0.00946 0.00130 0.00726 0.00050

287 4XY 0.00009 -0.00509 -0.00199 -0.00689 0.00031

288 4XZ -0.00061 0.01048 0.00223 0.00822 -0.00248

289 4YZ 0.00070 0.00607 0.00100 0.00318 0.00140

290 20 O 1S -0.00025 -0.00008 0.00045 0.00174 0.00506

291 2S 0.00088 -0.00125 -0.00131 -0.00439 -0.00949

292 2PX -0.00547 0.01074 -0.04395 -0.13121 0.03848

293 2PY -0.00425 0.00876 -0.02515 -0.07189 0.00388

294 2PZ -0.00127 -0.00008 -0.01839 -0.05672 0.03084

295 3S -0.00075 0.01025 -0.00202 -0.01218 -0.04975

296 3PX -0.00515 0.00932 -0.04591 -0.13906 0.03906

297 3PY -0.00447 0.01125 -0.02478 -0.07234 0.00375

298 3PZ -0.00148 -0.00068 -0.01976 -0.05821 0.03354

299 4XX -0.00029 0.00325 -0.00205 -0.00563 0.00335

300 4YY 0.00060 -0.00303 0.00275 0.00759 0.00050

301 4ZZ -0.00009 -0.00142 -0.00052 -0.00146 0.00027

302 4XY 0.00016 -0.00146 0.00197 0.00621 -0.00312

303 4XZ 0.00003 -0.00145 -0.00111 -0.00369 0.00210

304 4YZ -0.00002 -0.00177 0.00074 0.00230 -0.00169

305 21 O 1S -0.00063 0.00001 -0.00027 0.00051 -0.00190

306 2S 0.00131 0.00019 0.00041 -0.00148 0.00220

307 2PX 0.00440 -0.12961 0.01071 0.01953 -0.01314

308 2PY 0.00297 -0.06552 0.00488 0.00799 -0.01649

309 2PZ -0.00081 -0.05685 0.00186 0.00563 -0.03050

310 3S 0.00553 -0.00336 0.00325 -0.00198 0.02620

311 3PX 0.00491 -0.13653 0.00938 0.01336 -0.00580

312 3PY 0.00215 -0.06969 0.00288 0.00332 -0.02296

313 3PZ -0.00231 -0.06056 0.00029 0.00276 -0.04186

314 4XX 0.00009 -0.01082 0.00012 -0.00031 -0.00282

315 4YY -0.00035 0.00518 -0.00098 -0.00208 0.00029

316 4ZZ -0.00010 0.00568 0.00054 0.00230 0.00005

317 4XY -0.00013 0.00270 -0.00081 -0.00222 0.00120

318 4XZ -0.00005 0.00474 0.00075 0.00281 -0.00040

319 4YZ -0.00012 0.00611 0.00001 0.00060 0.00076

320 22 H 1S -0.00004 -0.00030 -0.00026 -0.00030 -0.00132

321 2S -0.00026 0.00080 -0.00157 -0.00186 -0.01082

322 23 H 1S 0.00023 -0.00062 -0.00017 -0.00041 -0.00170

323 2S 0.00023 -0.00613 -0.00112 -0.00062 -0.01081

324 24 H 1S 0.00063 0.00062 0.00093 0.00087 -0.00194

325 2S -0.00312 0.02053 -0.01406 -0.01716 -0.02969

326 25 H 1S -0.00032 0.00264 -0.00081 -0.00100 -0.00345

327 2S -0.00187 -0.00818 0.00129 0.00561 -0.02471

328 26 H 1S -0.00052 0.00131 -0.00055 -0.00027 -0.00370

329 2S -0.00147 0.00639 -0.00297 -0.00183 -0.01922

330 27 H 1S -0.00557 0.00301 -0.00364 -0.00402 -0.02440

331 2S -0.00549 0.00200 -0.01182 -0.01160 -0.12382

332 28 H 1S -0.00423 0.00272 -0.00259 -0.00266 -0.01963

333 2S -0.01775 0.01712 -0.01696 -0.01764 -0.14859

334 29 H 1S 0.00312 0.02731 0.00403 0.01584 0.00345

335 2S -0.01189 0.07477 -0.00082 0.02517 -0.01408

336 30 H 1S -0.00458 0.03545 0.00839 0.03217 -0.00645

337 2S -0.01927 0.05139 0.02873 0.11287 -0.02725

338 31 H 1S 0.00228 -0.06332 -0.01339 -0.05027 0.00201

339 2S -0.03839 -0.16650 -0.10998 -0.14827 -0.02236

340 32 H 1S -0.00041 0.00101 0.00028 0.00129 0.00652

341 2S -0.00233 0.00215 0.00224 0.00990 0.02898

342 33 H 1S -0.00084 -0.00069 -0.00056 0.00038 -0.00623

343 2S -0.00841 -0.00068 -0.00794 -0.00307 -0.07154

**Table S2.** Second order perturbation theory analysis of Fock Matrix in NBO basis of POTMBD using B3LYP/6-311++G(d,p).

E(2) E(j)-E(i) F(i,j)

Donor NBO (i) Acceptor NBO (j) kcal/mol a.u. a.u.

=====================================================================================

1. BD ( 1) C 1 - C 2 / 99. RY\*( 1) C 3 0.54 1.97 0.029

1. BD ( 1) C 1 - C 2 /100. RY\*( 2) C 3 1.61 1.47 0.044

1. BD ( 1) C 1 - C 2 /129. RY\*( 1) C 6 0.71 1.97 0.033

1. BD ( 1) C 1 - C 2 /130. RY\*( 2) C 6 1.41 1.40 0.040

1. BD ( 1) C 1 - C 2 /303. BD\*( 1) C 1 - C 6 2.38 1.27 0.049

1. BD ( 1) C 1 - C 2 /304. BD\*( 1) C 1 - H 22 1.10 1.17 0.032

1. BD ( 1) C 1 - C 2 /305. BD\*( 1) C 2 - C 3 2.54 1.28 0.051

1. BD ( 1) C 1 - C 2 /306. BD\*( 1) C 2 - H 23 1.14 1.17 0.033

1. BD ( 1) C 1 - C 2 /309. BD\*( 1) C 3 - H 24 2.31 1.17 0.046

1. BD ( 1) C 1 - C 2 /315. BD\*( 1) C 6 - H 26 2.28 1.17 0.046

2. BD ( 2) C 1 - C 2 /102. RY\*( 4) C 3 1.46 1.42 0.045

2. BD ( 2) C 1 - C 2 /132. RY\*( 4) C 6 1.15 0.98 0.033

2. BD ( 2) C 1 - C 2 /308. BD\*( 2) C 3 - C 4 21.31 0.28 0.069

2. BD ( 2) C 1 - C 2 /313. BD\*( 2) C 5 - C 6 18.85 0.28 0.066

3. BD ( 1) C 1 - C 6 / 89. RY\*( 1) C 2 0.66 1.96 0.032

3. BD ( 1) C 1 - C 6 / 90. RY\*( 2) C 2 1.47 1.40 0.041

3. BD ( 1) C 1 - C 6 /119. RY\*( 1) C 5 0.60 1.97 0.031

3. BD ( 1) C 1 - C 6 /120. RY\*( 2) C 5 1.55 1.48 0.043

3. BD ( 1) C 1 - C 6 /301. BD\*( 1) C 1 - C 2 2.39 1.27 0.049

3. BD ( 1) C 1 - C 6 /304. BD\*( 1) C 1 - H 22 1.09 1.16 0.032

3. BD ( 1) C 1 - C 6 /306. BD\*( 1) C 2 - H 23 2.33 1.16 0.047

3. BD ( 1) C 1 - C 6 /312. BD\*( 1) C 5 - C 6 2.52 1.28 0.051

3. BD ( 1) C 1 - C 6 /314. BD\*( 1) C 5 - H 25 2.30 1.18 0.047

3. BD ( 1) C 1 - C 6 /315. BD\*( 1) C 6 - H 26 1.11 1.17 0.032

4. BD ( 1) C 1 - H 22 / 89. RY\*( 1) C 2 1.11 1.79 0.040

4. BD ( 1) C 1 - H 22 /129. RY\*( 1) C 6 1.11 1.80 0.040

4. BD ( 1) C 1 - H 22 /301. BD\*( 1) C 1 - C 2 0.78 1.10 0.026

4. BD ( 1) C 1 - H 22 /303. BD\*( 1) C 1 - C 6 0.76 1.10 0.026

4. BD ( 1) C 1 - H 22 /305. BD\*( 1) C 2 - C 3 3.59 1.11 0.056

4. BD ( 1) C 1 - H 22 /312. BD\*( 1) C 5 - C 6 3.53 1.11 0.056

5. BD ( 1) C 2 - C 3 / 79. RY\*( 1) C 1 0.67 1.97 0.033

5. BD ( 1) C 2 - C 3 / 80. RY\*( 2) C 1 1.38 1.40 0.039

5. BD ( 1) C 2 - C 3 /109. RY\*( 1) C 4 1.50 2.10 0.050

5. BD ( 1) C 2 - C 3 /110. RY\*( 2) C 4 1.04 1.87 0.039

5. BD ( 1) C 2 - C 3 /301. BD\*( 1) C 1 - C 2 2.50 1.27 0.050

5. BD ( 1) C 2 - C 3 /304. BD\*( 1) C 1 - H 22 2.25 1.17 0.046

5. BD ( 1) C 2 - C 3 /306. BD\*( 1) C 2 - H 23 1.09 1.17 0.032

5. BD ( 1) C 2 - C 3 /307. BD\*( 1) C 3 - C 4 2.98 1.26 0.055

5. BD ( 1) C 2 - C 3 /309. BD\*( 1) C 3 - H 24 1.26 1.17 0.034

5. BD ( 1) C 2 - C 3 /311. BD\*( 1) C 4 - C 7 3.58 1.18 0.058

6. BD ( 1) C 2 - H 23 / 79. RY\*( 1) C 1 1.11 1.80 0.040

6. BD ( 1) C 2 - H 23 / 99. RY\*( 1) C 3 1.01 1.80 0.038

6. BD ( 1) C 2 - H 23 /301. BD\*( 1) C 1 - C 2 0.79 1.10 0.026

6. BD ( 1) C 2 - H 23 /303. BD\*( 1) C 1 - C 6 3.53 1.10 0.056

6. BD ( 1) C 2 - H 23 /305. BD\*( 1) C 2 - C 3 0.82 1.10 0.027

6. BD ( 1) C 2 - H 23 /307. BD\*( 1) C 3 - C 4 3.81 1.09 0.058

7. BD ( 1) C 3 - C 4 / 89. RY\*( 1) C 2 0.85 1.96 0.037

7. BD ( 1) C 3 - C 4 / 90. RY\*( 2) C 2 1.48 1.40 0.041

7. BD ( 1) C 3 - C 4 /139. RY\*( 1) C 7 0.85 1.56 0.033

7. BD ( 1) C 3 - C 4 /305. BD\*( 1) C 2 - C 3 2.38 1.28 0.049

7. BD ( 1) C 3 - C 4 /306. BD\*( 1) C 2 - H 23 2.17 1.17 0.045

7. BD ( 1) C 3 - C 4 /309. BD\*( 1) C 3 - H 24 1.10 1.17 0.032

7. BD ( 1) C 3 - C 4 /310. BD\*( 1) C 4 - C 5 4.04 1.26 0.064

7. BD ( 1) C 3 - C 4 /311. BD\*( 1) C 4 - C 7 2.31 1.18 0.047

7. BD ( 1) C 3 - C 4 /314. BD\*( 1) C 5 - H 25 1.94 1.18 0.043

7. BD ( 1) C 3 - C 4 /316. BD\*( 1) C 7 - N 8 2.74 1.26 0.053

8. BD ( 2) C 3 - C 4 / 92. RY\*( 4) C 2 1.29 0.97 0.035

8. BD ( 2) C 3 - C 4 /121. RY\*( 3) C 5 0.93 1.88 0.041

8. BD ( 2) C 3 - C 4 /143. RY\*( 5) C 7 0.66 2.05 0.036

8. BD ( 2) C 3 - C 4 /302. BD\*( 2) C 1 - C 2 19.23 0.28 0.066

8. BD ( 2) C 3 - C 4 /313. BD\*( 2) C 5 - C 6 19.24 0.29 0.067

8. BD ( 2) C 3 - C 4 /317. BD\*( 2) C 7 - N 8 22.06 0.26 0.069

9. BD ( 1) C 3 - H 24 / 89. RY\*( 1) C 2 1.14 1.79 0.040

9. BD ( 1) C 3 - H 24 /109. RY\*( 1) C 4 1.50 1.93 0.048

9. BD ( 1) C 3 - H 24 /301. BD\*( 1) C 1 - C 2 3.55 1.10 0.056

9. BD ( 1) C 3 - H 24 /305. BD\*( 1) C 2 - C 3 0.95 1.11 0.029

9. BD ( 1) C 3 - H 24 /307. BD\*( 1) C 3 - C 4 0.90 1.09 0.028

9. BD ( 1) C 3 - H 24 /310. BD\*( 1) C 4 - C 5 4.19 1.09 0.060

10. BD ( 1) C 4 - C 5 /129. RY\*( 1) C 6 0.80 1.96 0.036

10. BD ( 1) C 4 - C 5 /130. RY\*( 2) C 6 1.53 1.40 0.042

10. BD ( 1) C 4 - C 5 /139. RY\*( 1) C 7 1.19 1.55 0.039

10. BD ( 1) C 4 - C 5 /307. BD\*( 1) C 3 - C 4 4.02 1.25 0.063

10. BD ( 1) C 4 - C 5 /309. BD\*( 1) C 3 - H 24 2.14 1.16 0.045

10. BD ( 1) C 4 - C 5 /311. BD\*( 1) C 4 - C 7 2.49 1.17 0.048

10. BD ( 1) C 4 - C 5 /312. BD\*( 1) C 5 - C 6 2.27 1.28 0.048

10. BD ( 1) C 4 - C 5 /314. BD\*( 1) C 5 - H 25 1.06 1.18 0.032

10. BD ( 1) C 4 - C 5 /315. BD\*( 1) C 6 - H 26 2.23 1.16 0.046

10. BD ( 1) C 4 - C 5 /318. BD\*( 1) C 7 - O 11 3.41 1.01 0.053

11. BD ( 1) C 4 - C 7 / 99. RY\*( 1) C 3 1.62 1.98 0.051

11. BD ( 1) C 4 - C 7 /119. RY\*( 1) C 5 1.53 1.97 0.049

11. BD ( 1) C 4 - C 7 /149. RY\*( 1) N 8 0.69 1.76 0.031

11. BD ( 1) C 4 - C 7 /170. RY\*( 2) C 10 0.67 1.87 0.032

11. BD ( 1) C 4 - C 7 /305. BD\*( 1) C 2 - C 3 1.80 1.28 0.043

11. BD ( 1) C 4 - C 7 /307. BD\*( 1) C 3 - C 4 2.39 1.26 0.049

11. BD ( 1) C 4 - C 7 /310. BD\*( 1) C 4 - C 5 2.09 1.26 0.046

11. BD ( 1) C 4 - C 7 /312. BD\*( 1) C 5 - C 6 1.94 1.28 0.045

11. BD ( 1) C 4 - C 7 /316. BD\*( 1) C 7 - N 8 2.62 1.26 0.051

11. BD ( 1) C 4 - C 7 /319. BD\*( 1) N 8 - N 9 1.95 1.06 0.041

11. BD ( 1) C 4 - C 7 /322. BD\*( 1) C 10 - O 11 2.15 1.01 0.042

12. BD ( 1) C 5 - C 6 / 79. RY\*( 1) C 1 0.67 1.97 0.033

12. BD ( 1) C 5 - C 6 / 80. RY\*( 2) C 1 1.37 1.40 0.039

12. BD ( 1) C 5 - C 6 /109. RY\*( 1) C 4 0.97 2.10 0.040

12. BD ( 1) C 5 - C 6 /110. RY\*( 2) C 4 1.61 1.87 0.049

12. BD ( 1) C 5 - C 6 /303. BD\*( 1) C 1 - C 6 2.49 1.27 0.050

12. BD ( 1) C 5 - C 6 /304. BD\*( 1) C 1 - H 22 2.25 1.17 0.046

12. BD ( 1) C 5 - C 6 /310. BD\*( 1) C 4 - C 5 2.82 1.26 0.053

12. BD ( 1) C 5 - C 6 /311. BD\*( 1) C 4 - C 7 3.26 1.18 0.056

12. BD ( 1) C 5 - C 6 /314. BD\*( 1) C 5 - H 25 1.28 1.18 0.035

12. BD ( 1) C 5 - C 6 /315. BD\*( 1) C 6 - H 26 1.11 1.17 0.032

13. BD ( 2) C 5 - C 6 / 82. RY\*( 4) C 1 1.59 1.00 0.039

13. BD ( 2) C 5 - C 6 /114. RY\*( 6) C 4 0.59 1.82 0.032

13. BD ( 2) C 5 - C 6 /302. BD\*( 2) C 1 - C 2 20.73 0.28 0.068

13. BD ( 2) C 5 - C 6 /308. BD\*( 2) C 3 - C 4 19.59 0.28 0.067

14. BD ( 1) C 5 - H 25 /109. RY\*( 1) C 4 1.50 1.93 0.048

14. BD ( 1) C 5 - H 25 /129. RY\*( 1) C 6 1.11 1.79 0.040

14. BD ( 1) C 5 - H 25 /303. BD\*( 1) C 1 - C 6 3.62 1.09 0.056

14. BD ( 1) C 5 - H 25 /307. BD\*( 1) C 3 - C 4 4.26 1.08 0.061

14. BD ( 1) C 5 - H 25 /310. BD\*( 1) C 4 - C 5 0.91 1.08 0.028

14. BD ( 1) C 5 - H 25 /312. BD\*( 1) C 5 - C 6 0.99 1.11 0.030

15. BD ( 1) C 6 - H 26 / 79. RY\*( 1) C 1 1.10 1.80 0.040

15. BD ( 1) C 6 - H 26 /119. RY\*( 1) C 5 1.05 1.80 0.039

15. BD ( 1) C 6 - H 26 /301. BD\*( 1) C 1 - C 2 3.52 1.10 0.056

15. BD ( 1) C 6 - H 26 /303. BD\*( 1) C 1 - C 6 0.76 1.10 0.026

15. BD ( 1) C 6 - H 26 /310. BD\*( 1) C 4 - C 5 3.82 1.08 0.058

15. BD ( 1) C 6 - H 26 /312. BD\*( 1) C 5 - C 6 0.86 1.11 0.028

16. BD ( 1) C 7 - N 8 /110. RY\*( 2) C 4 0.93 2.06 0.039

16. BD ( 1) C 7 - N 8 /139. RY\*( 1) C 7 0.54 1.75 0.028

16. BD ( 1) C 7 - N 8 /160. RY\*( 2) N 9 1.10 2.06 0.043

16. BD ( 1) C 7 - N 8 /307. BD\*( 1) C 3 - C 4 1.33 1.45 0.039

16. BD ( 1) C 7 - N 8 /311. BD\*( 1) C 4 - C 7 3.10 1.36 0.058

16. BD ( 1) C 7 - N 8 /323. BD\*( 1) C 10 - S 12 1.15 1.07 0.032

17. BD ( 2) C 7 - N 8 /111. RY\*( 3) C 4 1.00 1.42 0.035

17. BD ( 2) C 7 - N 8 /161. RY\*( 3) N 9 0.94 1.26 0.032

17. BD ( 2) C 7 - N 8 /308. BD\*( 2) C 3 - C 4 8.73 0.36 0.054

17. BD ( 2) C 7 - N 8 /321. BD\*( 2) N 9 - C 10 10.78 0.32 0.055

18. BD ( 1) C 7 - O 11 /110. RY\*( 2) C 4 0.98 2.08 0.040

18. BD ( 1) C 7 - O 11 /139. RY\*( 1) C 7 0.52 1.77 0.027

18. BD ( 1) C 7 - O 11 /169. RY\*( 1) C 10 2.50 1.69 0.058

18. BD ( 1) C 7 - O 11 /310. BD\*( 1) C 4 - C 5 1.44 1.47 0.041

18. BD ( 1) C 7 - O 11 /322. BD\*( 1) C 10 - O 11 0.78 1.23 0.028

18. BD ( 1) C 7 - O 11 /323. BD\*( 1) C 10 - S 12 5.21 1.10 0.068

19. BD ( 1) N 8 - N 9 /139. RY\*( 1) C 7 0.60 1.63 0.028

19. BD ( 1) N 8 - N 9 /140. RY\*( 2) C 7 0.60 1.86 0.030

19. BD ( 1) N 8 - N 9 /169. RY\*( 1) C 10 0.83 1.54 0.032

19. BD ( 1) N 8 - N 9 /170. RY\*( 2) C 10 0.66 1.94 0.032

19. BD ( 1) N 8 - N 9 /311. BD\*( 1) C 4 - C 7 6.50 1.25 0.081

19. BD ( 1) N 8 - N 9 /318. BD\*( 1) C 7 - O 11 2.23 1.09 0.044

19. BD ( 1) N 8 - N 9 /322. BD\*( 1) C 10 - O 11 2.12 1.08 0.043

19. BD ( 1) N 8 - N 9 /323. BD\*( 1) C 10 - S 12 7.45 0.96 0.076

20. BD ( 1) N 9 - C 10 /140. RY\*( 2) C 7 0.57 1.99 0.030

20. BD ( 1) N 9 - C 10 /150. RY\*( 2) N 8 1.16 2.04 0.044

20. BD ( 1) N 9 - C 10 /311. BD\*( 1) C 4 - C 7 1.10 1.37 0.035

20. BD ( 1) N 9 - C 10 /323. BD\*( 1) C 10 - S 12 0.83 1.08 0.027

21. BD ( 2) N 9 - C 10 /151. RY\*( 3) N 8 1.04 2.09 0.043

21. BD ( 2) N 9 - C 10 /180. RY\*( 2) O 11 0.53 1.43 0.025

21. BD ( 2) N 9 - C 10 /190. RY\*( 2) S 12 1.20 0.89 0.030

21. BD ( 2) N 9 - C 10 /317. BD\*( 2) C 7 - N 8 10.13 0.34 0.056

21. BD ( 2) N 9 - C 10 /321. BD\*( 2) N 9 - C 10 0.59 0.33 0.013

22. BD ( 1) C 10 - O 11 /139. RY\*( 1) C 7 1.66 1.79 0.049

22. BD ( 1) C 10 - O 11 /311. BD\*( 1) C 4 - C 7 4.15 1.41 0.069

22. BD ( 1) C 10 - O 11 /318. BD\*( 1) C 7 - O 11 0.61 1.25 0.025

23. BD ( 1) C 10 - S 12 /140. RY\*( 2) C 7 0.75 1.77 0.033

23. BD ( 1) C 10 - S 12 /159. RY\*( 1) N 9 1.03 1.61 0.037

23. BD ( 1) C 10 - S 12 /179. RY\*( 1) O 11 0.63 1.91 0.031

23. BD ( 1) C 10 - S 12 /199. RY\*( 1) C 13 0.87 1.88 0.036

23. BD ( 1) C 10 - S 12 /201. RY\*( 3) C 13 0.62 1.57 0.028

23. BD ( 1) C 10 - S 12 /318. BD\*( 1) C 7 - O 11 2.25 1.00 0.043

23. BD ( 1) C 10 - S 12 /319. BD\*( 1) N 8 - N 9 2.72 1.04 0.048

23. BD ( 1) C 10 - S 12 /326. BD\*( 2) C 13 - C 14 1.24 0.69 0.029

24. BD ( 1) S 12 - C 13 /209. RY\*( 1) C 14 1.97 1.80 0.054

24. BD ( 1) S 12 - C 13 /249. RY\*( 1) C 18 2.37 1.84 0.059

24. BD ( 1) S 12 - C 13 /320. BD\*( 1) N 9 - C 10 3.10 1.19 0.054

24. BD ( 1) S 12 - C 13 /323. BD\*( 1) C 10 - S 12 0.66 0.82 0.021

24. BD ( 1) S 12 - C 13 /327. BD\*( 1) C 13 - C 18 0.66 1.18 0.025

24. BD ( 1) S 12 - C 13 /328. BD\*( 1) C 14 - C 15 3.21 1.20 0.056

24. BD ( 1) S 12 - C 13 /335. BD\*( 1) C 17 - C 18 3.01 1.19 0.053

25. BD ( 1) C 13 - C 14 /220. RY\*( 2) C 15 1.97 1.56 0.050

25. BD ( 1) C 13 - C 14 /249. RY\*( 1) C 18 1.66 1.92 0.051

25. BD ( 1) C 13 - C 14 /327. BD\*( 1) C 13 - C 18 4.14 1.26 0.065

25. BD ( 1) C 13 - C 14 /328. BD\*( 1) C 14 - C 15 2.66 1.28 0.052

25. BD ( 1) C 13 - C 14 /329. BD\*( 1) C 14 - H 27 1.43 1.18 0.037

25. BD ( 1) C 13 - C 14 /332. BD\*( 1) C 15 - H 28 2.29 1.16 0.046

25. BD ( 1) C 13 - C 14 /338. BD\*( 1) C 18 - C 19 3.27 1.13 0.054

26. BD ( 2) C 13 - C 14 /189. RY\*( 1) S 12 1.39 0.97 0.035

26. BD ( 2) C 13 - C 14 /222. RY\*( 4) C 15 0.86 0.95 0.028

26. BD ( 2) C 13 - C 14 /251. RY\*( 3) C 18 0.76 1.16 0.029

26. BD ( 2) C 13 - C 14 /323. BD\*( 1) C 10 - S 12 3.47 0.45 0.038

26. BD ( 2) C 13 - C 14 /331. BD\*( 2) C 15 - C 16 16.15 0.28 0.062

26. BD ( 2) C 13 - C 14 /336. BD\*( 2) C 17 - C 18 19.19 0.29 0.069

27. BD ( 1) C 13 - C 18 /209. RY\*( 1) C 14 1.05 1.88 0.040

27. BD ( 1) C 13 - C 18 /210. RY\*( 2) C 14 0.54 1.48 0.025

27. BD ( 1) C 13 - C 18 /239. RY\*( 1) C 17 1.04 1.68 0.037

27. BD ( 1) C 13 - C 18 /259. RY\*( 1) C 19 0.56 1.49 0.026

27. BD ( 1) C 13 - C 18 /325. BD\*( 1) C 13 - C 14 3.79 1.27 0.062

27. BD ( 1) C 13 - C 18 /329. BD\*( 1) C 14 - H 27 1.89 1.18 0.042

27. BD ( 1) C 13 - C 18 /335. BD\*( 1) C 17 - C 18 2.96 1.27 0.055

27. BD ( 1) C 13 - C 18 /337. BD\*( 1) C 17 - O 20 3.57 1.06 0.055

27. BD ( 1) C 13 - C 18 /338. BD\*( 1) C 18 - C 19 2.42 1.13 0.047

28. BD ( 1) C 14 - C 15 /199. RY\*( 1) C 13 0.81 1.90 0.035

28. BD ( 1) C 14 - C 15 /200. RY\*( 2) C 13 1.57 1.53 0.044

28. BD ( 1) C 14 - C 15 /230. RY\*( 2) C 16 1.83 1.90 0.053

28. BD ( 1) C 14 - C 15 /324. BD\*( 1) S 12 - C 13 3.75 0.88 0.051

28. BD ( 1) C 14 - C 15 /325. BD\*( 1) C 13 - C 14 3.04 1.26 0.055

28. BD ( 1) C 14 - C 15 /329. BD\*( 1) C 14 - H 27 1.11 1.17 0.032

28. BD ( 1) C 14 - C 15 /330. BD\*( 1) C 15 - C 16 2.81 1.26 0.053

28. BD ( 1) C 14 - C 15 /332. BD\*( 1) C 15 - H 28 1.43 1.15 0.036

28. BD ( 1) C 14 - C 15 /334. BD\*( 1) C 16 - O 21 5.08 1.03 0.065

29. BD ( 1) C 14 - H 27 /199. RY\*( 1) C 13 1.30 1.73 0.042

29. BD ( 1) C 14 - H 27 /219. RY\*( 1) C 15 0.80 1.66 0.033

29. BD ( 1) C 14 - H 27 /325. BD\*( 1) C 13 - C 14 1.18 1.09 0.032

29. BD ( 1) C 14 - H 27 /327. BD\*( 1) C 13 - C 18 4.14 1.08 0.060

29. BD ( 1) C 14 - H 27 /328. BD\*( 1) C 14 - C 15 0.92 1.10 0.028

29. BD ( 1) C 14 - H 27 /330. BD\*( 1) C 15 - C 16 3.61 1.09 0.056

30. BD ( 1) C 15 - C 16 /210. RY\*( 2) C 14 2.22 1.50 0.052

30. BD ( 1) C 15 - C 16 /240. RY\*( 2) C 17 1.88 1.78 0.052

30. BD ( 1) C 15 - C 16 /328. BD\*( 1) C 14 - C 15 2.74 1.30 0.053

30. BD ( 1) C 15 - C 16 /329. BD\*( 1) C 14 - H 27 2.13 1.20 0.045

30. BD ( 1) C 15 - C 16 /332. BD\*( 1) C 15 - H 28 1.15 1.17 0.033

30. BD ( 1) C 15 - C 16 /333. BD\*( 1) C 16 - C 17 3.97 1.26 0.063

30. BD ( 1) C 15 - C 16 /337. BD\*( 1) C 17 - O 20 3.04 1.08 0.051

31. BD ( 2) C 15 - C 16 /213. RY\*( 5) C 14 1.02 1.67 0.040

31. BD ( 2) C 15 - C 16 /279. RY\*( 1) O 21 1.04 1.26 0.035

31. BD ( 2) C 15 - C 16 /326. BD\*( 2) C 13 - C 14 21.35 0.29 0.072

31. BD ( 2) C 15 - C 16 /336. BD\*( 2) C 17 - C 18 17.17 0.30 0.065

32. BD ( 1) C 15 - H 28 /209. RY\*( 1) C 14 1.07 1.71 0.038

32. BD ( 1) C 15 - H 28 /230. RY\*( 2) C 16 0.67 1.74 0.030

32. BD ( 1) C 15 - H 28 /325. BD\*( 1) C 13 - C 14 3.54 1.10 0.056

32. BD ( 1) C 15 - H 28 /328. BD\*( 1) C 14 - C 15 1.10 1.11 0.031

32. BD ( 1) C 15 - H 28 /330. BD\*( 1) C 15 - C 16 0.77 1.10 0.026

32. BD ( 1) C 15 - H 28 /333. BD\*( 1) C 16 - C 17 4.34 1.07 0.061

32. BD ( 1) C 15 - H 28 /334. BD\*( 1) C 16 - O 21 0.57 0.87 0.020

33. BD ( 1) C 16 - C 17 /219. RY\*( 1) C 15 1.25 1.86 0.043

33. BD ( 1) C 16 - C 17 /250. RY\*( 2) C 18 2.65 1.75 0.061

33. BD ( 1) C 16 - C 17 /280. RY\*( 2) O 21 0.77 2.01 0.035

33. BD ( 1) C 16 - C 17 /330. BD\*( 1) C 15 - C 16 3.48 1.28 0.060

33. BD ( 1) C 16 - C 17 /332. BD\*( 1) C 15 - H 28 2.17 1.17 0.045

33. BD ( 1) C 16 - C 17 /335. BD\*( 1) C 17 - C 18 3.70 1.28 0.062

33. BD ( 1) C 16 - C 17 /338. BD\*( 1) C 18 - C 19 2.68 1.14 0.050

33. BD ( 1) C 16 - C 17 /343. BD\*( 1) O 21 - H 33 2.01 1.12 0.043

34. BD ( 1) C 16 - O 21 /328. BD\*( 1) C 14 - C 15 1.13 1.49 0.037

34. BD ( 1) C 16 - O 21 /330. BD\*( 1) C 15 - C 16 0.92 1.48 0.033

34. BD ( 1) C 16 - O 21 /335. BD\*( 1) C 17 - C 18 1.94 1.48 0.048

35. BD ( 1) C 17 - C 18 /199. RY\*( 1) C 13 0.82 1.91 0.036

35. BD ( 1) C 17 - C 18 /200. RY\*( 2) C 13 0.80 1.54 0.032

35. BD ( 1) C 17 - C 18 /229. RY\*( 1) C 16 1.74 1.65 0.048

35. BD ( 1) C 17 - C 18 /259. RY\*( 1) C 19 0.74 1.48 0.030

35. BD ( 1) C 17 - C 18 /270. RY\*( 2) O 20 0.52 1.97 0.029

35. BD ( 1) C 17 - C 18 /324. BD\*( 1) S 12 - C 13 4.19 0.89 0.054

35. BD ( 1) C 17 - C 18 /327. BD\*( 1) C 13 - C 18 3.47 1.26 0.059

35. BD ( 1) C 17 - C 18 /333. BD\*( 1) C 16 - C 17 3.31 1.24 0.057

35. BD ( 1) C 17 - C 18 /334. BD\*( 1) C 16 - O 21 2.70 1.03 0.047

35. BD ( 1) C 17 - C 18 /337. BD\*( 1) C 17 - O 20 0.58 1.06 0.022

35. BD ( 1) C 17 - C 18 /338. BD\*( 1) C 18 - C 19 1.56 1.13 0.038

35. BD ( 1) C 17 - C 18 /339. BD\*( 1) C 19 - H 29 0.73 1.17 0.026

35. BD ( 1) C 17 - C 18 /342. BD\*( 1) O 20 - H 32 1.74 1.13 0.040

36. BD ( 2) C 17 - C 18 /236. RY\*( 8) C 16 0.77 0.96 0.027

36. BD ( 2) C 17 - C 18 /269. RY\*( 1) O 20 1.25 1.27 0.039

36. BD ( 2) C 17 - C 18 /326. BD\*( 2) C 13 - C 14 18.22 0.27 0.064

36. BD ( 2) C 17 - C 18 /331. BD\*( 2) C 15 - C 16 22.87 0.28 0.072

36. BD ( 2) C 17 - C 18 /340. BD\*( 1) C 19 - H 30 0.73 0.72 0.023

36. BD ( 2) C 17 - C 18 /341. BD\*( 1) C 19 - H 31 2.46 0.71 0.041

37. BD ( 1) C 17 - O 20 /249. RY\*( 1) C 18 0.64 2.11 0.033

37. BD ( 1) C 17 - O 20 /327. BD\*( 1) C 13 - C 18 1.73 1.46 0.045

37. BD ( 1) C 17 - O 20 /330. BD\*( 1) C 15 - C 16 1.61 1.47 0.044

37. BD ( 1) C 17 - O 20 /333. BD\*( 1) C 16 - C 17 0.65 1.44 0.027

37. BD ( 1) C 17 - O 20 /335. BD\*( 1) C 17 - C 18 1.08 1.47 0.036

38. BD ( 1) C 18 - C 19 /199. RY\*( 1) C 13 1.36 1.82 0.045

38. BD ( 1) C 18 - C 19 /239. RY\*( 1) C 17 1.07 1.59 0.037

38. BD ( 1) C 18 - C 19 /325. BD\*( 1) C 13 - C 14 2.36 1.18 0.047

38. BD ( 1) C 18 - C 19 /327. BD\*( 1) C 13 - C 18 2.66 1.17 0.050

38. BD ( 1) C 18 - C 19 /333. BD\*( 1) C 16 - C 17 3.21 1.15 0.055

38. BD ( 1) C 18 - C 19 /335. BD\*( 1) C 17 - C 18 2.10 1.18 0.045

38. BD ( 1) C 18 - C 19 /339. BD\*( 1) C 19 - H 29 0.54 1.08 0.022

38. BD ( 1) C 18 - C 19 /340. BD\*( 1) C 19 - H 30 0.52 1.08 0.021

38. BD ( 1) C 18 - C 19 /341. BD\*( 1) C 19 - H 31 0.52 1.07 0.021

39. BD ( 1) C 19 - H 29 /250. RY\*( 2) C 18 0.51 1.52 0.025

39. BD ( 1) C 19 - H 29 /335. BD\*( 1) C 17 - C 18 3.55 1.06 0.055

39. BD ( 1) C 19 - H 29 /336. BD\*( 2) C 17 - C 18 0.63 0.53 0.018

39. BD ( 1) C 19 - H 29 /338. BD\*( 1) C 18 - C 19 0.57 0.92 0.020

40. BD ( 1) C 19 - H 30 /327. BD\*( 1) C 13 - C 18 3.53 1.05 0.054

40. BD ( 1) C 19 - H 30 /336. BD\*( 2) C 17 - C 18 1.37 0.52 0.026

40. BD ( 1) C 19 - H 30 /338. BD\*( 1) C 18 - C 19 0.52 0.91 0.020

41. BD ( 1) C 19 - H 31 /251. RY\*( 3) C 18 1.08 1.39 0.035

41. BD ( 1) C 19 - H 31 /327. BD\*( 1) C 13 - C 18 0.91 1.04 0.028

41. BD ( 1) C 19 - H 31 /336. BD\*( 2) C 17 - C 18 4.07 0.52 0.045

42. BD ( 1) O 20 - H 32 /239. RY\*( 1) C 17 1.39 1.71 0.044

42. BD ( 1) O 20 - H 32 /335. BD\*( 1) C 17 - C 18 5.32 1.30 0.075

43. BD ( 1) O 21 - H 33 /229. RY\*( 1) C 16 1.05 1.71 0.038

43. BD ( 1) O 21 - H 33 /333. BD\*( 1) C 16 - C 17 4.27 1.30 0.067

44. CR ( 1) C 1 / 90. RY\*( 2) C 2 1.53 10.76 0.115

44. CR ( 1) C 1 /130. RY\*( 2) C 6 1.56 10.76 0.116

44. CR ( 1) C 1 /305. BD\*( 1) C 2 - C 3 0.73 10.64 0.079

44. CR ( 1) C 1 /306. BD\*( 1) C 2 - H 23 0.66 10.53 0.075

44. CR ( 1) C 1 /312. BD\*( 1) C 5 - C 6 0.72 10.64 0.078

44. CR ( 1) C 1 /315. BD\*( 1) C 6 - H 26 0.65 10.53 0.074

45. CR ( 1) C 2 / 80. RY\*( 2) C 1 1.63 10.75 0.118

45. CR ( 1) C 2 /100. RY\*( 2) C 3 1.25 10.83 0.104

45. CR ( 1) C 2 /103. RY\*( 5) C 3 0.55 11.23 0.070

45. CR ( 1) C 2 /303. BD\*( 1) C 1 - C 6 0.70 10.63 0.077

45. CR ( 1) C 2 /304. BD\*( 1) C 1 - H 22 0.65 10.52 0.074

45. CR ( 1) C 2 /307. BD\*( 1) C 3 - C 4 0.80 10.62 0.083

45. CR ( 1) C 2 /309. BD\*( 1) C 3 - H 24 0.67 10.53 0.075

46. CR ( 1) C 3 / 90. RY\*( 2) C 2 1.73 10.76 0.122

46. CR ( 1) C 3 /110. RY\*( 2) C 4 1.71 11.23 0.124

46. CR ( 1) C 3 /301. BD\*( 1) C 1 - C 2 0.73 10.63 0.079

46. CR ( 1) C 3 /306. BD\*( 1) C 2 - H 23 0.63 10.53 0.073

46. CR ( 1) C 3 /310. BD\*( 1) C 4 - C 5 0.90 10.62 0.088

46. CR ( 1) C 3 /311. BD\*( 1) C 4 - C 7 0.96 10.53 0.090

47. CR ( 1) C 4 /100. RY\*( 2) C 3 1.45 10.84 0.112

47. CR ( 1) C 4 /120. RY\*( 2) C 5 1.39 10.85 0.110

47. CR ( 1) C 4 /142. RY\*( 4) C 7 1.05 12.06 0.101

47. CR ( 1) C 4 /305. BD\*( 1) C 2 - C 3 0.61 10.64 0.072

47. CR ( 1) C 4 /309. BD\*( 1) C 3 - H 24 0.62 10.54 0.072

47. CR ( 1) C 4 /312. BD\*( 1) C 5 - C 6 0.60 10.65 0.072

47. CR ( 1) C 4 /314. BD\*( 1) C 5 - H 25 0.57 10.55 0.070

47. CR ( 1) C 4 /316. BD\*( 1) C 7 - N 8 1.08 10.63 0.096

47. CR ( 1) C 4 /318. BD\*( 1) C 7 - O 11 0.66 10.38 0.075

48. CR ( 1) C 5 /109. RY\*( 1) C 4 0.66 11.46 0.077

48. CR ( 1) C 5 /110. RY\*( 2) C 4 1.25 11.22 0.106

48. CR ( 1) C 5 /130. RY\*( 2) C 6 1.70 10.76 0.121

48. CR ( 1) C 5 /292. RY\*( 1) H 25 0.50 10.66 0.065

48. CR ( 1) C 5 /303. BD\*( 1) C 1 - C 6 0.75 10.62 0.080

48. CR ( 1) C 5 /307. BD\*( 1) C 3 - C 4 0.93 10.61 0.089

48. CR ( 1) C 5 /311. BD\*( 1) C 4 - C 7 0.88 10.53 0.087

48. CR ( 1) C 5 /315. BD\*( 1) C 6 - H 26 0.63 10.52 0.073

49. CR ( 1) C 6 / 80. RY\*( 2) C 1 1.61 10.75 0.117

49. CR ( 1) C 6 /120. RY\*( 2) C 5 1.38 10.84 0.109

49. CR ( 1) C 6 /123. RY\*( 5) C 5 0.53 11.25 0.069

49. CR ( 1) C 6 /301. BD\*( 1) C 1 - C 2 0.70 10.63 0.077

49. CR ( 1) C 6 /304. BD\*( 1) C 1 - H 22 0.65 10.52 0.074

49. CR ( 1) C 6 /310. BD\*( 1) C 4 - C 5 0.79 10.61 0.082

49. CR ( 1) C 6 /314. BD\*( 1) C 5 - H 25 0.67 10.54 0.075

50. CR ( 1) C 7 /109. RY\*( 1) C 4 1.17 11.56 0.104

50. CR ( 1) C 7 /150. RY\*( 2) N 8 1.14 11.31 0.101

50. CR ( 1) C 7 /307. BD\*( 1) C 3 - C 4 0.74 10.72 0.080

50. CR ( 1) C 7 /310. BD\*( 1) C 4 - C 5 0.62 10.72 0.073

50. CR ( 1) C 7 /318. BD\*( 1) C 7 - O 11 1.03 10.47 0.094

50. CR ( 1) C 7 /322. BD\*( 1) C 10 - O 11 1.17 10.47 0.100

51. CR ( 1) N 8 /139. RY\*( 1) C 7 3.85 15.04 0.215

51. CR ( 1) N 8 /311. BD\*( 1) C 4 - C 7 1.30 14.65 0.124

51. CR ( 1) N 8 /319. BD\*( 1) N 8 - N 9 0.59 14.53 0.083

51. CR ( 1) N 8 /320. BD\*( 1) N 9 - C 10 0.60 14.73 0.085

52. CR ( 1) N 9 /169. RY\*( 1) C 10 4.10 14.94 0.222

52. CR ( 1) N 9 /316. BD\*( 1) C 7 - N 8 0.57 14.73 0.082

52. CR ( 1) N 9 /319. BD\*( 1) N 8 - N 9 0.65 14.53 0.087

52. CR ( 1) N 9 /323. BD\*( 1) C 10 - S 12 1.40 14.36 0.128

53. CR ( 1) C 10 /160. RY\*( 2) N 9 1.22 11.38 0.105

53. CR ( 1) C 10 /318. BD\*( 1) C 7 - O 11 1.21 10.51 0.102

53. CR ( 1) C 10 /320. BD\*( 1) N 9 - C 10 0.79 10.75 0.083

54. CR ( 1) O 11 /139. RY\*( 1) C 7 1.46 19.87 0.153

54. CR ( 1) O 11 /140. RY\*( 2) C 7 0.93 20.10 0.122

54. CR ( 1) O 11 /169. RY\*( 1) C 10 1.88 19.78 0.173

54. CR ( 1) O 11 /170. RY\*( 2) C 10 0.95 20.18 0.124

54. CR ( 1) O 11 /323. BD\*( 1) C 10 - S 12 0.54 19.20 0.092

56. CR ( 2) S 12 /170. RY\*( 2) C 10 0.58 10.14 0.068

56. CR ( 2) S 12 /171. RY\*( 3) C 10 0.57 10.34 0.069

56. CR ( 2) S 12 /199. RY\*( 1) C 13 0.79 10.17 0.080

56. CR ( 2) S 12 /320. BD\*( 1) N 9 - C 10 0.99 9.52 0.087

56. CR ( 2) S 12 /322. BD\*( 1) C 10 - O 11 1.09 9.28 0.091

56. CR ( 2) S 12 /325. BD\*( 1) C 13 - C 14 0.51 9.53 0.063

56. CR ( 2) S 12 /327. BD\*( 1) C 13 - C 18 0.76 9.52 0.077

60. CR ( 1) C 13 /210. RY\*( 2) C 14 1.98 10.86 0.131

60. CR ( 1) C 13 /250. RY\*( 2) C 18 2.20 11.12 0.140

60. CR ( 1) C 13 /324. BD\*( 1) S 12 - C 13 1.40 10.27 0.108

60. CR ( 1) C 13 /325. BD\*( 1) C 13 - C 14 0.68 10.65 0.077

60. CR ( 1) C 13 /327. BD\*( 1) C 13 - C 18 0.62 10.64 0.073

60. CR ( 1) C 13 /328. BD\*( 1) C 14 - C 15 0.71 10.66 0.078

60. CR ( 1) C 13 /329. BD\*( 1) C 14 - H 27 0.66 10.56 0.075

60. CR ( 1) C 13 /335. BD\*( 1) C 17 - C 18 0.68 10.65 0.077

60. CR ( 1) C 13 /338. BD\*( 1) C 18 - C 19 1.05 10.51 0.094

61. CR ( 1) C 14 /200. RY\*( 2) C 13 2.00 10.89 0.132

61. CR ( 1) C 14 /219. RY\*( 1) C 15 0.89 11.19 0.089

61. CR ( 1) C 14 /220. RY\*( 2) C 15 0.63 10.90 0.074

61. CR ( 1) C 14 /223. RY\*( 5) C 15 0.52 11.27 0.068

61. CR ( 1) C 14 /324. BD\*( 1) S 12 - C 13 1.08 10.23 0.094

61. CR ( 1) C 14 /325. BD\*( 1) C 13 - C 14 0.56 10.62 0.069

61. CR ( 1) C 14 /327. BD\*( 1) C 13 - C 18 1.07 10.61 0.096

61. CR ( 1) C 14 /330. BD\*( 1) C 15 - C 16 0.75 10.62 0.080

61. CR ( 1) C 14 /332. BD\*( 1) C 15 - H 28 0.71 10.50 0.077

62. CR ( 1) C 15 /209. RY\*( 1) C 14 0.76 11.23 0.083

62. CR ( 1) C 15 /210. RY\*( 2) C 14 1.00 10.83 0.093

62. CR ( 1) C 15 /212. RY\*( 4) C 14 0.52 11.27 0.068

62. CR ( 1) C 15 /229. RY\*( 1) C 16 1.86 11.01 0.128

62. CR ( 1) C 15 /325. BD\*( 1) C 13 - C 14 0.80 10.62 0.083

62. CR ( 1) C 15 /329. BD\*( 1) C 14 - H 27 0.63 10.53 0.073

62. CR ( 1) C 15 /333. BD\*( 1) C 16 - C 17 1.04 10.59 0.095

62. CR ( 1) C 15 /334. BD\*( 1) C 16 - O 21 1.07 10.39 0.094

63. CR ( 1) C 16 /220. RY\*( 2) C 15 1.70 10.98 0.122

63. CR ( 1) C 16 /239. RY\*( 1) C 17 1.44 11.10 0.113

63. CR ( 1) C 16 /328. BD\*( 1) C 14 - C 15 0.61 10.70 0.073

63. CR ( 1) C 16 /330. BD\*( 1) C 15 - C 16 0.88 10.69 0.087

63. CR ( 1) C 16 /332. BD\*( 1) C 15 - H 28 0.69 10.58 0.076

63. CR ( 1) C 16 /333. BD\*( 1) C 16 - C 17 0.78 10.66 0.082

63. CR ( 1) C 16 /334. BD\*( 1) C 16 - O 21 1.41 10.46 0.109

63. CR ( 1) C 16 /335. BD\*( 1) C 17 - C 18 0.95 10.69 0.090

63. CR ( 1) C 16 /337. BD\*( 1) C 17 - O 20 0.67 10.49 0.075

64. CR ( 1) C 17 /230. RY\*( 2) C 16 1.55 11.32 0.118

64. CR ( 1) C 17 /249. RY\*( 1) C 18 1.43 11.33 0.114

64. CR ( 1) C 17 /250. RY\*( 2) C 18 0.72 11.15 0.080

64. CR ( 1) C 17 /327. BD\*( 1) C 13 - C 18 0.80 10.67 0.083

64. CR ( 1) C 17 /330. BD\*( 1) C 15 - C 16 0.95 10.68 0.091

64. CR ( 1) C 17 /333. BD\*( 1) C 16 - C 17 0.61 10.65 0.072

64. CR ( 1) C 17 /334. BD\*( 1) C 16 - O 21 0.54 10.45 0.068

64. CR ( 1) C 17 /335. BD\*( 1) C 17 - C 18 1.10 10.68 0.097

64. CR ( 1) C 17 /337. BD\*( 1) C 17 - O 20 1.26 10.47 0.103

64. CR ( 1) C 17 /338. BD\*( 1) C 18 - C 19 0.76 10.54 0.080

65. CR ( 1) C 18 /200. RY\*( 2) C 13 2.00 10.89 0.132

65. CR ( 1) C 18 /240. RY\*( 2) C 17 1.78 11.11 0.126

65. CR ( 1) C 18 /261. RY\*( 3) C 19 0.64 11.07 0.075

65. CR ( 1) C 18 /324. BD\*( 1) S 12 - C 13 1.18 10.24 0.099

65. CR ( 1) C 18 /325. BD\*( 1) C 13 - C 14 0.87 10.62 0.086

65. CR ( 1) C 18 /327. BD\*( 1) C 13 - C 18 0.57 10.61 0.070

65. CR ( 1) C 18 /333. BD\*( 1) C 16 - C 17 1.03 10.59 0.094

65. CR ( 1) C 18 /337. BD\*( 1) C 17 - O 20 0.75 10.41 0.079

66. CR ( 1) C 19 /249. RY\*( 1) C 18 0.96 11.26 0.093

66. CR ( 1) C 19 /296. RY\*( 1) H 29 0.50 10.75 0.066

66. CR ( 1) C 19 /327. BD\*( 1) C 13 - C 18 0.82 10.60 0.084

66. CR ( 1) C 19 /335. BD\*( 1) C 17 - C 18 0.58 10.61 0.071

67. CR ( 1) O 20 /239. RY\*( 1) C 17 1.97 19.96 0.177

67. CR ( 1) O 20 /240. RY\*( 2) C 17 0.51 20.04 0.090

68. CR ( 1) O 21 /229. RY\*( 1) C 16 1.62 19.96 0.161

68. CR ( 1) O 21 /230. RY\*( 2) C 16 0.59 20.21 0.098

68. CR ( 1) O 21 /234. RY\*( 6) C 16 0.66 20.97 0.105

68. CR ( 1) O 21 /330. BD\*( 1) C 15 - C 16 0.62 19.58 0.099

69. LP ( 1) N 8 /139. RY\*( 1) C 7 5.92 1.26 0.078

69. LP ( 1) N 8 /140. RY\*( 2) C 7 1.13 1.49 0.037

69. LP ( 1) N 8 /159. RY\*( 1) N 9 1.79 1.33 0.044

69. LP ( 1) N 8 /318. BD\*( 1) C 7 - O 11 11.28 0.71 0.080

69. LP ( 1) N 8 /320. BD\*( 1) N 9 - C 10 4.85 0.95 0.061

70. LP ( 1) N 9 /149. RY\*( 1) N 8 1.97 1.46 0.049

70. LP ( 1) N 9 /169. RY\*( 1) C 10 6.58 1.17 0.079

70. LP ( 1) N 9 /170. RY\*( 2) C 10 1.40 1.57 0.043

70. LP ( 1) N 9 /316. BD\*( 1) C 7 - N 8 4.86 0.96 0.062

70. LP ( 1) N 9 /322. BD\*( 1) C 10 - O 11 10.77 0.71 0.078

71. LP ( 1) O 11 /139. RY\*( 1) C 7 1.76 1.47 0.046

71. LP ( 1) O 11 /140. RY\*( 2) C 7 2.09 1.70 0.054

71. LP ( 1) O 11 /169. RY\*( 1) C 10 2.16 1.38 0.049

71. LP ( 1) O 11 /170. RY\*( 2) C 10 2.54 1.78 0.060

71. LP ( 1) O 11 /316. BD\*( 1) C 7 - N 8 4.19 1.18 0.063

71. LP ( 1) O 11 /320. BD\*( 1) N 9 - C 10 4.16 1.17 0.062

72. LP ( 2) O 11 /141. RY\*( 3) C 7 1.15 2.32 0.050

72. LP ( 2) O 11 /143. RY\*( 5) C 7 0.55 2.15 0.033

72. LP ( 2) O 11 /173. RY\*( 5) C 10 1.58 2.43 0.060

72. LP ( 2) O 11 /317. BD\*( 2) C 7 - N 8 32.37 0.36 0.097

72. LP ( 2) O 11 /321. BD\*( 2) N 9 - C 10 33.69 0.34 0.097

73. LP ( 1) S 12 /170. RY\*( 2) C 10 0.77 1.80 0.033

73. LP ( 1) S 12 /171. RY\*( 3) C 10 0.63 2.00 0.032

73. LP ( 1) S 12 /199. RY\*( 1) C 13 0.95 1.83 0.037

73. LP ( 1) S 12 /322. BD\*( 1) C 10 - O 11 5.41 0.94 0.064

73. LP ( 1) S 12 /326. BD\*( 2) C 13 - C 14 1.10 0.64 0.026

73. LP ( 1) S 12 /327. BD\*( 1) C 13 - C 18 1.75 1.18 0.041

74. LP ( 2) S 12 /200. RY\*( 2) C 13 0.78 1.08 0.027

74. LP ( 2) S 12 /320. BD\*( 1) N 9 - C 10 0.88 0.81 0.025

74. LP ( 2) S 12 /321. BD\*( 2) N 9 - C 10 23.12 0.24 0.070

74. LP ( 2) S 12 /322. BD\*( 1) C 10 - O 11 1.17 0.57 0.023

74. LP ( 2) S 12 /325. BD\*( 1) C 13 - C 14 3.71 0.81 0.051

74. LP ( 2) S 12 /326. BD\*( 2) C 13 - C 14 0.55 0.27 0.012

74. LP ( 2) S 12 /327. BD\*( 1) C 13 - C 18 3.80 0.80 0.051

74. LP ( 2) S 12 /328. BD\*( 1) C 14 - C 15 0.62 0.82 0.021

74. LP ( 2) S 12 /339. BD\*( 1) C 19 - H 29 1.27 0.71 0.028

75. LP ( 1) O 20 /239. RY\*( 1) C 17 3.02 1.57 0.062

75. LP ( 1) O 20 /242. RY\*( 4) C 17 0.65 2.55 0.037

75. LP ( 1) O 20 /333. BD\*( 1) C 16 - C 17 6.13 1.13 0.075

76. LP ( 2) O 20 /241. RY\*( 3) C 17 2.08 2.21 0.063

76. LP ( 2) O 20 /245. RY\*( 7) C 17 0.62 1.16 0.025

76. LP ( 2) O 20 /336. BD\*( 2) C 17 - C 18 27.11 0.35 0.093

77. LP ( 1) O 21 /229. RY\*( 1) C 16 2.68 1.57 0.058

77. LP ( 1) O 21 /232. RY\*( 4) C 16 0.54 2.44 0.033

77. LP ( 1) O 21 /330. BD\*( 1) C 15 - C 16 6.19 1.18 0.076

77. LP ( 1) O 21 /333. BD\*( 1) C 16 - C 17 0.51 1.15 0.022

77. LP ( 1) O 21 /342. BD\*( 1) O 20 - H 32 2.94 1.04 0.049

78. LP ( 2) O 21 /231. RY\*( 3) C 16 2.00 2.26 0.062

78. LP ( 2) O 21 /331. BD\*( 2) C 15 - C 16 25.83 0.36 0.093

302. BD\*( 2) C 1 - C 2 / 82. RY\*( 4) C 1 1.51 0.72 0.073

302. BD\*( 2) C 1 - C 2 / 92. RY\*( 4) C 2 2.15 0.69 0.085

308. BD\*( 2) C 3 - C 4 /101. RY\*( 3) C 3 1.43 1.40 0.091

308. BD\*( 2) C 3 - C 4 /113. RY\*( 5) C 4 0.53 1.83 0.063

308. BD\*( 2) C 3 - C 4 /114. RY\*( 6) C 4 0.59 1.54 0.061

313. BD\*( 2) C 5 - C 6 /122. RY\*( 4) C 5 2.00 0.96 0.101

313. BD\*( 2) C 5 - C 6 /132. RY\*( 4) C 6 2.11 0.70 0.089

317. BD\*( 2) C 7 - N 8 /144. RY\*( 6) C 7 0.98 1.38 0.085

317. BD\*( 2) C 7 - N 8 /153. RY\*( 5) N 8 1.67 0.95 0.092

317. BD\*( 2) C 7 - N 8 /308. BD\*( 2) C 3 - C 4 117.20 0.02 0.072

321. BD\*( 2) N 9 - C 10 /161. RY\*( 3) N 9 0.90 0.94 0.064

321. BD\*( 2) N 9 - C 10 /171. RY\*( 3) C 10 0.54 1.38 0.060

321. BD\*( 2) N 9 - C 10 /172. RY\*( 4) C 10 1.16 1.36 0.087

321. BD\*( 2) N 9 - C 10 /190. RY\*( 2) S 12 0.64 0.56 0.042

321. BD\*( 2) N 9 - C 10 /317. BD\*( 2) C 7 - N 8 70.70 0.02 0.056

326. BD\*( 2) C 13 - C 14 /211. RY\*( 3) C 14 2.36 1.11 0.101

326. BD\*( 2) C 13 - C 14 /323. BD\*( 1) C 10 - S 12 2.02 0.17 0.035

326. BD\*( 2) C 13 - C 14 /336. BD\*( 2) C 17 - C 18 216.04 0.01 0.079

331. BD\*( 2) C 15 - C 16 /222. RY\*( 4) C 15 3.26 0.67 0.093

331. BD\*( 2) C 15 - C 16 /231. RY\*( 3) C 16 0.55 1.90 0.064

331. BD\*( 2) C 15 - C 16 /236. RY\*( 8) C 16 0.86 0.69 0.048

331. BD\*( 2) C 15 - C 16 /279. RY\*( 1) O 21 0.54 0.97 0.045

331. BD\*( 2) C 15 - C 16 /336. BD\*( 2) C 17 - C 18 249.74 0.01 0.082

336. BD\*( 2) C 17 - C 18 /241. RY\*( 3) C 17 0.55 1.86 0.066

336. BD\*( 2) C 17 - C 18 /245. RY\*( 7) C 17 0.91 0.81 0.056

336. BD\*( 2) C 17 - C 18 /255. RY\*( 7) C 18 0.86 1.70 0.079

336. BD\*( 2) C 17 - C 18 /269. RY\*( 1) O 20 0.51 0.98 0.046

336. BD\*( 2) C 17 - C 18 /340. BD\*( 1) C 19 - H 30 0.66 0.43 0.034

336. BD\*( 2) C 17 - C 18 /341. BD\*( 1) C 19 - H 31 1.53 0.42 0.052

**Table S3.** Summary of Bond Orbitals of POTMBD using B3LYP/6-311++G(d,p).

Principal Delocalizations

NBO Occupancy Energy (geminal,vicinal,remote)

====================================================================================

Molecular unit 1 (C15H12N2O3S)

1. BD ( 1) C 1 - C 2 1.98132 -0.69470 305(g),303(g),309(v),315(v)

100(v),130(v),306(g),304(g)

129(v),99(v)

2. BD ( 2) C 1 - C 2 1.65266 -0.24979 308(v),313(v),102(v),132(v)

3. BD ( 1) C 1 - C 6 1.98136 -0.69285 312(g),301(g),306(v),314(v)

120(v),90(v),315(g),304(g)

89(v),119(v)

4. BD ( 1) C 1 - H 22 1.98313 -0.52508 305(v),312(v),129(v),89(v)

301(g),303(g)

5. BD ( 1) C 2 - C 3 1.97993 -0.69640 311(v),307(g),301(g),304(v)

109(v),80(v),309(g),306(g)

110(v),79(v)

6. BD ( 1) C 2 - H 23 1.98251 -0.52432 307(v),303(v),79(v),99(v)

305(g),301(g)

7. BD ( 1) C 3 - C 4 1.97444 -0.69612 310(g),316(v),305(g),311(g)

306(v),314(v),90(v),309(g)

89(v),139(v)

8. BD ( 2) C 3 - C 4 1.64231 -0.25222 317(v),313(v),302(v),92(v)

121(v),143(v)

9. BD ( 1) C 3 - H 24 1.98170 -0.52577 310(v),301(v),109(v),89(v)

305(g),307(g)

10. BD ( 1) C 4 - C 5 1.97076 -0.69008 307(g),318(v),311(g),312(g)

315(v),309(v),130(v),139(v)

314(g),129(v)

11. BD ( 1) C 4 - C 7 1.97289 -0.69560 316(g),307(g),322(v),310(g)

319(v),312(v),305(v),99(v)

119(v),149(v),170(r)

12. BD ( 1) C 5 - C 6 1.98000 -0.69612 311(v),310(g),303(g),304(v)

110(v),80(v),314(g),315(g)

109(v),79(v)

13. BD ( 2) C 5 - C 6 1.66291 -0.24944 302(v),308(v),82(v),114(v)

14. BD ( 1) C 5 - H 25 1.98089 -0.51886 307(v),303(v),109(v),129(v)

312(g),310(g)

15. BD ( 1) C 6 - H 26 1.98237 -0.52255 310(v),301(v),79(v),119(v)

312(g),303(g)

16. BD ( 1) C 7 - N 8 1.99284 -0.88312 311(g),307(v),323(r),160(v)

110(v),139(g)

17. BD ( 2) C 7 - N 8 1.88671 -0.32712 321(v),308(v),111(v),161(v)

18. BD ( 1) C 7 - O 11 1.98477 -0.91023 323(v),169(v),310(v),110(v)

322(g),139(g)

19. BD ( 1) N 8 - N 9 1.96291 -0.76866 323(v),311(v),318(v),322(v)

169(v),170(v),140(v),139(v)

20. BD ( 1) N 9 - C 10 1.99505 -0.89375 150(v),311(r),323(g),140(r)

21. BD ( 2) N 9 - C 10 1.90309 -0.33512 317(v),190(v),151(v),321(g)

180(v)

22. BD ( 1) C 10 - O 11 1.99038 -0.93004 311(v),139(v),318(g)

23. BD ( 1) C 10 - S 12 1.97102 -0.67920 319(v),318(v),326(v),159(v)

199(v),140(r),179(v),201(v)

24. BD ( 1) S 12 - C 13 1.97118 -0.62955 328(v),320(v),335(v),249(v)

209(v),323(g),327(g)

25. BD ( 1) C 13 - C 14 1.97847 -0.71280 327(g),338(v),328(g),332(v)

220(v),249(v),329(g)

26. BD ( 2) C 13 - C 14 1.71902 -0.26516 336(v),331(v),323(v),189(v)

222(v),251(v)

27. BD ( 1) C 13 - C 18 1.97410 -0.70867 325(g),337(v),335(g),338(g)

329(v),209(v),239(v),259(v)

210(v)

28. BD ( 1) C 14 - C 15 1.97026 -0.70240 334(v),324(v),325(g),330(g)

230(v),200(v),332(g),329(g)

199(v)

29. BD ( 1) C 14 - H 27 1.98055 -0.52826 327(v),330(v),199(v),325(g)

328(g),219(v)

30. BD ( 1) C 15 - C 16 1.97907 -0.72856 333(g),337(v),328(g),210(v)

329(v),240(v),332(g)

31. BD ( 2) C 15 - C 16 1.69165 -0.27375 326(v),336(v),279(v),213(v)

32. BD ( 1) C 15 - H 28 1.97798 -0.54192 333(v),325(v),328(g),209(v)

330(g),230(v),334(v)

33. BD ( 1) C 16 - C 17 1.97382 -0.72315 335(g),330(g),338(v),250(v)

332(v),343(v),219(v),280(v)

34. BD ( 1) C 16 - O 21 1.99438 -0.92080 335(v),328(v),330(g)

35. BD ( 1) C 17 - C 18 1.96574 -0.70763 324(v),327(g),333(g),334(v)

229(v),342(v),338(g),199(v)

200(v),259(v),339(v),337(g)

270(v)

36. BD ( 2) C 17 - C 18 1.63870 -0.25994 331(v),326(v),341(v),269(v)

236(v),340(v)

37. BD ( 1) C 17 - O 20 1.99330 -0.90571 327(v),330(v),335(g),333(g)

249(v)

38. BD ( 1) C 18 - C 19 1.98037 -0.62132 333(v),327(g),325(v),335(g)

199(v),239(v),339(g),341(g)

340(g)

39. BD ( 1) C 19 - H 29 1.98672 -0.49784 335(v),336(v),338(g),250(v)

40. BD ( 1) C 19 - H 30 1.98399 -0.49445 327(v),336(v),338(g)

41. BD ( 1) C 19 - H 31 1.97486 -0.49271 336(v),251(v),327(v)

42. BD ( 1) O 20 - H 32 1.98795 -0.73864 335(v),239(v)

43. BD ( 1) O 21 - H 33 1.98923 -0.76309 333(v),229(v)

44. CR ( 1) C 1 1.99910 -10.05442 130(v),90(v),305(v),312(v)

306(v),315(v)

45. CR ( 1) C 2 1.99911 -10.05326 80(v),100(v),307(v),303(v)

309(v),304(v),103(v)

46. CR ( 1) C 3 1.99907 -10.05397 90(v),110(v),311(v),310(v)

301(v),306(v)

47. CR ( 1) C 4 1.99894 -10.06344 100(v),120(v),316(v),142(v)

318(v),309(v),305(v),312(v)

314(v)

48. CR ( 1) C 5 1.99907 -10.05083 130(v),110(v),307(v),311(v)

303(v),109(v),315(v),292(v)

49. CR ( 1) C 6 1.99911 -10.05217 80(v),120(v),310(v),301(v)

314(v),304(v),123(v)

50. CR ( 1) C 7 1.99915 -10.15645 322(v),109(v),150(v),318(g)

307(v),310(v)

51. CR ( 1) N 8 1.99941 -14.17197 139(v),311(v),320(v),319(g)

52. CR ( 1) N 9 1.99937 -14.16793 169(v),323(v),319(g),316(v)

53. CR ( 1) C 10 1.99922 -10.19651 318(v),160(v),320(g),322(g)

54. CR ( 1) O 11 1.99970 -19.00710 169(v),139(v),170(v),140(v)

323(v)

55. CR ( 1) S 12 2.00000 -87.65756

56. CR ( 2) S 12 1.99931 -8.96475 322(v),320(v),199(v),327(v)

170(v),171(v),325(v)

57. CR ( 3) S 12 1.99986 -5.92589

58. CR ( 4) S 12 1.99989 -5.92272

59. CR ( 5) S 12 1.99995 -5.91862

60. CR ( 1) C 13 1.99869 -10.09230 250(v),210(v),324(g),338(v)

328(v),325(g),335(v),329(v)

327(g)

61. CR ( 1) C 14 1.99899 -10.05501 200(v),324(v),327(v),219(v)

330(v),332(v),220(v),325(g)

223(v)

62. CR ( 1) C 15 1.99900 -10.06137 229(v),334(v),333(v),210(v)

325(v),209(v),329(v),212(v)

63. CR ( 1) C 16 1.99871 -10.13253 220(v),239(v),334(g),335(v)

330(g),333(g),332(v),337(v)

328(v)

64. CR ( 1) C 17 1.99864 -10.12147 230(v),249(v),337(g),335(g)

330(v),327(v),338(v),250(v)

333(g),334(v)

65. CR ( 1) C 18 1.99887 -10.06201 200(v),240(v),324(v),333(v)

325(v),337(v),261(v),327(g)

66. CR ( 1) C 19 1.99938 -10.04973 249(v),327(v),335(v),296(v)

67. CR ( 1) O 20 1.99978 -18.98607 239(v),240(v),333(v)

68. CR ( 1) O 21 1.99977 -19.01581 229(v),234(v),330(v),230(v)

69. LP ( 1) N 8 1.93240 -0.39431 318(v),139(v),320(v),159(v)

140(v)

70. LP ( 1) N 9 1.93515 -0.39279 322(v),169(v),316(v),149(v)

170(v)

71. LP ( 1) O 11 1.96864 -0.60907 316(v),320(v),170(v),169(v)

140(v),139(v)

72. LP ( 2) O 11 1.71284 -0.35178 321(v),317(v),173(v),141(v)

143(v)

73. LP ( 1) S 12 1.96740 -0.62792 322(v),327(v),326(v),199(v)

170(v),171(v)

74. LP ( 2) S 12 1.84082 -0.25057 321(v),327(v),325(v),339(r)

322(v),320(v),200(v),328(r)

326(v)

75. LP ( 1) O 20 1.97676 -0.59734 333(v),239(v),242(v)

76. LP ( 2) O 20 1.87030 -0.31976 336(v),241(v),245(v)

77. LP ( 1) O 21 1.97263 -0.62149 330(v),342(r),229(v),232(v)

333(v)

78. LP ( 2) O 21 1.88798 -0.34412 331(v),231(v)

79. RY\*( 1) C 1 0.00473 1.27271

80. RY\*( 2) C 1 0.00266 0.70064

81. RY\*( 3) C 1 0.00062 1.88521

82. RY\*( 4) C 1 0.00047 0.75506

83. RY\*( 5) C 1 0.00021 1.12040

84. RY\*( 6) C 1 0.00010 2.35762

85. RY\*( 7) C 1 0.00005 3.40112

86. RY\*( 8) C 1 0.00001 2.13190

87. RY\*( 9) C 1 0.00000 1.70368

88. RY\*( 10) C 1 0.00001 3.02625

89. RY\*( 1) C 2 0.00486 1.26616

90. RY\*( 2) C 2 0.00288 0.70692

91. RY\*( 3) C 2 0.00062 1.94034

92. RY\*( 4) C 2 0.00039 0.72237

93. RY\*( 5) C 2 0.00027 1.13192

94. RY\*( 6) C 2 0.00010 2.35814

95. RY\*( 7) C 2 0.00005 3.45519

96. RY\*( 8) C 2 0.00001 2.20054

97. RY\*( 9) C 2 0.00000 1.71030

98. RY\*( 10) C 2 0.00001 2.89680

99. RY\*( 1) C 3 0.00475 1.27954

100. RY\*( 2) C 3 0.00271 0.77931

101. RY\*( 3) C 3 0.00073 1.42806

102. RY\*( 4) C 3 0.00048 1.17228

103. RY\*( 5) C 3 0.00028 1.17863

104. RY\*( 6) C 3 0.00009 2.43852

105. RY\*( 7) C 3 0.00004 3.51822

106. RY\*( 8) C 3 0.00005 2.21144

107. RY\*( 9) C 3 0.00001 1.79322

108. RY\*( 10) C 3 0.00001 2.83308

109. RY\*( 1) C 4 0.00560 1.40723

110. RY\*( 2) C 4 0.00489 1.17331

111. RY\*( 3) C 4 0.00102 1.09290

112. RY\*( 4) C 4 0.00084 1.17242

113. RY\*( 5) C 4 0.00071 1.85771

114. RY\*( 6) C 4 0.00030 1.56800

115. RY\*( 7) C 4 0.00014 2.45243

116. RY\*( 8) C 4 0.00012 2.88149

117. RY\*( 9) C 4 0.00005 3.17699

118. RY\*( 10) C 4 0.00002 2.77347

119. RY\*( 1) C 5 0.00475 1.27694

120. RY\*( 2) C 5 0.00282 0.78741

121. RY\*( 3) C 5 0.00064 1.62302

122. RY\*( 4) C 5 0.00042 0.99620

123. RY\*( 5) C 5 0.00027 1.19418

124. RY\*( 6) C 5 0.00009 2.42924

125. RY\*( 7) C 5 0.00005 3.37921

126. RY\*( 8) C 5 0.00005 2.26703

127. RY\*( 9) C 5 0.00001 1.78218

128. RY\*( 10) C 5 0.00001 2.92679

129. RY\*( 1) C 6 0.00482 1.27049

130. RY\*( 2) C 6 0.00285 0.70908

131. RY\*( 3) C 6 0.00061 1.93962

132. RY\*( 4) C 6 0.00036 0.73104

133. RY\*( 5) C 6 0.00026 1.13380

134. RY\*( 6) C 6 0.00010 2.36401

135. RY\*( 7) C 6 0.00005 3.47774

136. RY\*( 8) C 6 0.00000 1.70703

137. RY\*( 9) C 6 0.00001 2.19716

138. RY\*( 10) C 6 0.00001 2.87542

139. RY\*( 1) C 7 0.01319 0.86402

140. RY\*( 2) C 7 0.00567 1.09357

141. RY\*( 3) C 7 0.00169 1.96804

142. RY\*( 4) C 7 0.00143 1.99419

143. RY\*( 5) C 7 0.00099 1.80066

144. RY\*( 6) C 7 0.00087 1.38700

145. RY\*( 7) C 7 0.00081 2.12952

146. RY\*( 8) C 7 0.00058 2.14176

147. RY\*( 9) C 7 0.00029 3.45651

148. RY\*( 10) C 7 0.00001 2.39449

149. RY\*( 1) N 8 0.00328 1.06743

150. RY\*( 2) N 8 0.00170 1.15048

151. RY\*( 3) N 8 0.00083 1.75859

152. RY\*( 4) N 8 0.00039 1.92572

153. RY\*( 5) N 8 0.00033 0.95701

154. RY\*( 6) N 8 0.00011 2.01929

155. RY\*( 7) N 8 0.00003 2.57309

156. RY\*( 8) N 8 0.00003 1.84779

157. RY\*( 9) N 8 0.00004 2.12585

158. RY\*( 10) N 8 0.00001 3.55682

159. RY\*( 1) N 9 0.00362 0.93387

160. RY\*( 2) N 9 0.00204 1.17974

161. RY\*( 3) N 9 0.00096 0.93135

162. RY\*( 4) N 9 0.00067 1.84318

163. RY\*( 5) N 9 0.00061 1.84016

164. RY\*( 6) N 9 0.00033 1.46911

165. RY\*( 7) N 9 0.00005 1.88463

166. RY\*( 8) N 9 0.00006 2.31329

167. RY\*( 9) N 9 0.00003 2.30898

168. RY\*( 10) N 9 0.00001 3.71672

169. RY\*( 1) C 10 0.01565 0.77556

170. RY\*( 2) C 10 0.00655 1.17570

171. RY\*( 3) C 10 0.00248 1.37441

172. RY\*( 4) C 10 0.00217 1.35010

173. RY\*( 5) C 10 0.00167 2.08077

174. RY\*( 6) C 10 0.00083 2.28343

175. RY\*( 7) C 10 0.00054 2.66523

176. RY\*( 8) C 10 0.00027 2.86475

177. RY\*( 9) C 10 0.00016 1.78555

178. RY\*( 10) C 10 0.00002 2.37038

179. RY\*( 1) O 11 0.00235 1.22839

180. RY\*( 2) O 11 0.00084 1.09866

181. RY\*( 3) O 11 0.00071 1.48171

182. RY\*( 4) O 11 0.00055 1.95307

183. RY\*( 5) O 11 0.00028 1.87770

184. RY\*( 6) O 11 0.00026 1.77097

185. RY\*( 7) O 11 0.00009 1.82353

186. RY\*( 8) O 11 0.00008 2.24711

187. RY\*( 9) O 11 0.00003 3.78446

188. RY\*( 10) O 11 0.00002 2.12721

189. RY\*( 1) S 12 0.00700 0.70364

190. RY\*( 2) S 12 0.00385 0.55644

191. RY\*( 3) S 12 0.00212 0.79627

192. RY\*( 4) S 12 0.00085 0.79664

193. RY\*( 5) S 12 0.00067 0.75716

194. RY\*( 6) S 12 0.00034 0.73566

195. RY\*( 7) S 12 0.00008 1.11502

196. RY\*( 8) S 12 0.00006 0.94513

197. RY\*( 9) S 12 0.00003 0.82262

198. RY\*( 10) S 12 0.00000 3.87934

199. RY\*( 1) C 13 0.00731 1.20050

200. RY\*( 2) C 13 0.00610 0.83101

201. RY\*( 3) C 13 0.00198 0.88606

202. RY\*( 4) C 13 0.00079 1.92350

203. RY\*( 5) C 13 0.00059 1.40469

204. RY\*( 6) C 13 0.00045 2.28420

205. RY\*( 7) C 13 0.00015 1.90468

206. RY\*( 8) C 13 0.00009 1.75194

207. RY\*( 9) C 13 0.00005 3.36565

208. RY\*( 10) C 13 0.00001 3.14645

209. RY\*( 1) C 14 0.00584 1.17167

210. RY\*( 2) C 14 0.00345 0.77070

211. RY\*( 3) C 14 0.00112 1.12370

212. RY\*( 4) C 14 0.00079 1.20461

213. RY\*( 5) C 14 0.00052 1.39365

214. RY\*( 6) C 14 0.00008 2.32856

215. RY\*( 7) C 14 0.00005 3.66484

216. RY\*( 8) C 14 0.00003 2.19213

217. RY\*( 9) C 14 0.00002 2.06387

218. RY\*( 10) C 14 0.00001 2.52625

219. RY\*( 1) C 15 0.00410 1.13546

220. RY\*( 2) C 15 0.00299 0.84417

221. RY\*( 3) C 15 0.00068 1.90139

222. RY\*( 4) C 15 0.00056 0.68734

223. RY\*( 5) C 15 0.00036 1.21545

224. RY\*( 6) C 15 0.00007 2.31751

225. RY\*( 7) C 15 0.00005 3.51613

226. RY\*( 8) C 15 0.00002 2.83453

227. RY\*( 9) C 15 0.00002 1.91680

228. RY\*( 10) C 15 0.00003 2.08479

229. RY\*( 1) C 16 0.00675 0.94634

230. RY\*( 2) C 16 0.00305 1.19556

231. RY\*( 3) C 16 0.00219 1.91787

232. RY\*( 4) C 16 0.00113 1.82136

233. RY\*( 5) C 16 0.00078 1.89099

234. RY\*( 6) C 16 0.00043 1.94978

235. RY\*( 7) C 16 0.00031 1.94043

236. RY\*( 8) C 16 0.00026 0.70392

237. RY\*( 9) C 16 0.00010 3.89156

238. RY\*( 10) C 16 0.00002 2.38413

239. RY\*( 1) C 17 0.00699 0.97010

240. RY\*( 2) C 17 0.00401 1.05125

241. RY\*( 3) C 17 0.00245 1.89150

242. RY\*( 4) C 17 0.00145 1.95093

243. RY\*( 5) C 17 0.00059 1.90309

244. RY\*( 6) C 17 0.00051 1.95450

245. RY\*( 7) C 17 0.00026 0.83605

246. RY\*( 8) C 17 0.00022 1.98018

247. RY\*( 9) C 17 0.00008 3.90986

248. RY\*( 10) C 17 0.00003 2.38565

249. RY\*( 1) C 18 0.00559 1.20911

250. RY\*( 2) C 18 0.00427 1.02599

251. RY\*( 3) C 18 0.00206 0.89512

252. RY\*( 4) C 18 0.00080 1.08378

253. RY\*( 5) C 18 0.00060 1.91748

254. RY\*( 6) C 18 0.00029 2.40337

255. RY\*( 7) C 18 0.00017 1.73074

256. RY\*( 8) C 18 0.00007 2.39105

257. RY\*( 9) C 18 0.00006 3.74227

258. RY\*( 10) C 18 0.00002 2.74333

259. RY\*( 1) C 19 0.00289 0.77688

260. RY\*( 2) C 19 0.00100 0.84056

261. RY\*( 3) C 19 0.00069 1.00792

262. RY\*( 4) C 19 0.00012 1.65328

263. RY\*( 5) C 19 0.00008 1.87943

264. RY\*( 6) C 19 0.00006 1.58655

265. RY\*( 7) C 19 0.00001 4.17291

266. RY\*( 8) C 19 0.00001 2.11078

267. RY\*( 9) C 19 0.00001 2.03888

268. RY\*( 10) C 19 0.00001 1.87245

269. RY\*( 1) O 20 0.00167 1.00908

270. RY\*( 2) O 20 0.00131 1.26557

271. RY\*( 3) O 20 0.00016 1.79100

272. RY\*( 4) O 20 0.00010 1.50690

273. RY\*( 5) O 20 0.00006 1.92631

274. RY\*( 6) O 20 0.00003 3.66345

275. RY\*( 7) O 20 0.00001 2.14926

276. RY\*( 8) O 20 0.00002 2.41601

277. RY\*( 9) O 20 0.00001 1.95057

278. RY\*( 10) O 20 0.00001 2.16928

279. RY\*( 1) O 21 0.00162 0.99000

280. RY\*( 2) O 21 0.00152 1.28324

281. RY\*( 3) O 21 0.00019 1.93761

282. RY\*( 4) O 21 0.00012 1.16596

283. RY\*( 5) O 21 0.00003 3.74313

284. RY\*( 6) O 21 0.00003 2.12612

285. RY\*( 7) O 21 0.00002 1.90134

286. RY\*( 8) O 21 0.00001 2.17071

287. RY\*( 9) O 21 0.00001 2.02938

288. RY\*( 10) O 21 0.00001 2.11662

289. RY\*( 1) H 22 0.00081 0.55827

290. RY\*( 1) H 23 0.00081 0.55799

291. RY\*( 1) H 24 0.00108 0.60956

292. RY\*( 1) H 25 0.00125 0.60447

293. RY\*( 1) H 26 0.00080 0.56045

294. RY\*( 1) H 27 0.00098 0.57270

295. RY\*( 1) H 28 0.00098 0.56111

296. RY\*( 1) H 29 0.00115 0.70333

297. RY\*( 1) H 30 0.00111 0.67106

298. RY\*( 1) H 31 0.00117 0.68451

299. RY\*( 1) H 32 0.00194 0.62911

300. RY\*( 1) H 33 0.00133 0.57893

301. BD\*( 1) C 1 - C 2 0.01564 0.57563

302. BD\*( 2) C 1 - C 2 0.32708 0.03112 308(v),313(v),92(g),82(g)

303. BD\*( 1) C 1 - C 6 0.01578 0.57347

304. BD\*( 1) C 1 - H 22 0.01200 0.47165

305. BD\*( 1) C 2 - C 3 0.01432 0.58067

306. BD\*( 1) C 2 - H 23 0.01194 0.47128

307. BD\*( 1) C 3 - C 4 0.02180 0.56386

308. BD\*( 2) C 3 - C 4 0.38683 0.02855 302(v),313(v),317(v),101(g)

114(g),113(g)

309. BD\*( 1) C 3 - H 24 0.01224 0.47451

310. BD\*( 1) C 4 - C 5 0.02170 0.56229

311. BD\*( 1) C 4 - C 7 0.03282 0.48047

312. BD\*( 1) C 5 - C 6 0.01411 0.58708

313. BD\*( 2) C 5 - C 6 0.29694 0.03514 302(v),308(v),132(g),122(g)

314. BD\*( 1) C 5 - H 25 0.01226 0.48534

315. BD\*( 1) C 6 - H 26 0.01201 0.47369

316. BD\*( 1) C 7 - N 8 0.02683 0.56664

317. BD\*( 2) C 7 - N 8 0.29529 0.00956 308(v),321(v),153(g),144(g)

318. BD\*( 1) C 7 - O 11 0.05780 0.31710

319. BD\*( 1) N 8 - N 9 0.01375 0.36165

320. BD\*( 1) N 9 - C 10 0.02992 0.55614

321. BD\*( 2) N 9 - C 10 0.32714 -0.00761 317(v),172(g),161(g),190(v)

171(g)

322. BD\*( 1) C 10 - O 11 0.06917 0.31531

323. BD\*( 1) C 10 - S 12 0.04704 0.18906

324. BD\*( 1) S 12 - C 13 0.02861 0.17850

325. BD\*( 1) C 13 - C 14 0.02406 0.56049

326. BD\*( 2) C 13 - C 14 0.40747 0.01501 331(v),336(v),211(g),323(v)

327. BD\*( 1) C 13 - C 18 0.03475 0.55135

328. BD\*( 1) C 14 - C 15 0.01714 0.57174

329. BD\*( 1) C 14 - H 27 0.01193 0.47163

330. BD\*( 1) C 15 - C 16 0.02430 0.56173

331. BD\*( 2) C 15 - C 16 0.40543 0.01573 326(v),336(v),222(g),236(g)

231(g),279(v)

332. BD\*( 1) C 15 - H 28 0.01246 0.44428

333. BD\*( 1) C 16 - C 17 0.03718 0.53222

334. BD\*( 1) C 16 - O 21 0.02250 0.32541

335. BD\*( 1) C 17 - C 18 0.02974 0.56075

336. BD\*( 2) C 17 - C 18 0.37453 0.02903 331(v),326(v),341(v),245(g)

255(g),340(v),241(g),269(v)

337. BD\*( 1) C 17 - O 20 0.01806 0.35251

338. BD\*( 1) C 18 - C 19 0.01474 0.41871

339. BD\*( 1) C 19 - H 29 0.00896 0.46132

340. BD\*( 1) C 19 - H 30 0.00806 0.46090

341. BD\*( 1) C 19 - H 31 0.00964 0.44864

342. BD\*( 1) O 20 - H 32 0.01445 0.41799

343. BD\*( 1) O 21 - H 33 0.00793 0.39585

-------------------------------

Total Lewis 152.15428 ( 97.5348%)

Valence non-Lewis 3.58634 ( 2.2989%)

Rydberg non-Lewis 0.25938 ( 0.1663%)

-------------------------------

Total unit 1 156.00000 (100.0000%)

Charge unit 1 0.00000

**Table S4.** Summary of Natural Population Analysis of POTMBD using B3LYP/6-311++G(d,p).

Natural Population

Natural -----------------------------------------------

Atom No Charge Core Valence Rydberg Total

-----------------------------------------------------------------------

C 1 -0.22214 1.99910 4.20957 0.01348 6.22214

C 2 -0.23141 1.99910 4.21850 0.01381 6.23141

C 3 -0.20539 1.99907 4.19364 0.01269 6.20539

C 4 -0.12896 1.99895 4.11516 0.01485 6.12896

C 5 -0.18945 1.99906 4.17757 0.01282 6.18945

C 6 -0.23123 1.99910 4.21842 0.01370 6.23123

C 7 0.50539 1.99915 3.46394 0.03152 5.49461

N 8 -0.29783 1.99940 5.27373 0.02469 7.29783

N 9 -0.32021 1.99937 5.29279 0.02806 7.32021

C 10 0.32065 1.99921 3.64137 0.03877 5.67935

O 11 -0.48665 1.99971 6.46929 0.01766 8.48665

S 12 0.34663 9.99901 5.61217 0.04219 15.65337

C 13 -0.22461 1.99869 4.20334 0.02258 6.22461

C 14 -0.22804 1.99898 4.21278 0.01627 6.22804

C 15 -0.30466 1.99900 4.29255 0.01311 6.30466

C 16 0.27384 1.99871 3.70774 0.01972 5.72616

C 17 0.29259 1.99864 3.68740 0.02137 5.70741

C 18 -0.05311 1.99887 4.03833 0.01591 6.05311

C 19 -0.69769 1.99938 4.68976 0.00855 6.69769

O 20 -0.69197 1.99978 6.68057 0.01161 8.69197

O 21 -0.71315 1.99977 6.70220 0.01118 8.71315

H 22 0.23923 0.00000 0.75996 0.00081 0.76077

H 23 0.24051 0.00000 0.75868 0.00081 0.75949

H 24 0.24888 0.00000 0.75005 0.00107 0.75112

H 25 0.25941 0.00000 0.73935 0.00124 0.74059

H 26 0.24190 0.00000 0.75730 0.00080 0.75810

H 27 0.25453 0.00000 0.74449 0.00097 0.74547

H 28 0.23785 0.00000 0.76117 0.00098 0.76215

H 29 0.25029 0.00000 0.74856 0.00115 0.74971

H 30 0.25588 0.00000 0.74300 0.00111 0.74412

H 31 0.25179 0.00000 0.74704 0.00117 0.74821

H 32 0.50504 0.00000 0.49305 0.00190 0.49496

H 33 0.50208 0.00000 0.49660 0.00132 0.49792

=======================================================================

\* Total \* 0.00000 49.98204 105.60007 0.41789 156.00000

Table S5: LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER along with STATISTICAL MECHANICAL ANALYSIS

RMSD cluster analysis will be performed using the ligand atoms only (23 / 23 total atoms).

Outputting structurally similar clusters, ranked in order of increasing energy.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Number of distinct conformational clusters found = 10, out of 10 runs,

Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

| | | | |

Clus | Lowest | Run | Mean | Num | Histogram

-ter | Binding | | Binding | in |

Rank | Energy | | Energy | Clus| 5 10 15 20 25 30 35

\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_|\_\_\_\_:\_\_\_\_|\_\_\_\_:\_\_\_\_|\_\_\_\_:\_\_\_\_|\_\_\_\_:\_\_\_

1 | -6.65 | 7 | -6.65 | 1 |#

2 | -6.13 | 10 | -6.13 | 1 |#

3 | -6.12 | 6 | -6.12 | 1 |#

4 | -5.73 | 8 | -5.73 | 1 |#

5 | -5.27 | 3 | -5.27 | 1 |#

6 | -5.03 | 4 | -5.03 | 1 |#

7 | -4.47 | 5 | -4.47 | 1 |#

8 | -4.44 | 2 | -4.44 | 1 |#

9 | -4.38 | 1 | -4.38 | 1 |#

10 | -4.12 | 9 | -4.12 | 1 |#

\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

RMSD TABLE

\_\_\_\_\_\_\_\_\_\_

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

| | | | | |

Rank | Sub- | Run | Binding | Cluster | Reference | Grep

| Rank | | Energy | RMSD | RMSD | Pattern

\_\_\_\_\_|\_\_\_\_\_\_|\_\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_|\_\_\_\_\_\_\_\_\_\_\_

1 1 7 -6.65 0.00 13.55 RANKING

2 1 10 -6.13 0.00 51.59 RANKING

3 1 6 -6.12 0.00 13.17 RANKING

4 1 8 -5.73 0.00 7.65 RANKING

5 1 3 -5.27 0.00 17.16 RANKING

6 1 4 -5.03 0.00 41.48 RANKING

7 1 5 -4.47 0.00 23.52 RANKING

8 1 2 -4.44 0.00 31.02 RANKING

9 1 1 -4.38 0.00 25.44 RANKING

10 1 9 -4.12 0.00 19.69 RANKING

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Information entropy for this clustering = 1.00 (rmstol = 2.00 Angstrom)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

STATISTICAL MECHANICAL ANALYSIS

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Partition function, Q = 10.09 at Temperature, T = 298.15 K

Free energy, A ~ -1369.47 kcal/mol at Temperature, T = 298.15 K

Internal energy, U = -5.24 kcal/mol at Temperature, T = 298.15 K

Entropy, S = 4.58 kcal/mol/K at Temperature, T = 298.15 K

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL 7

USER Run = 7

USER Cluster Rank = 1

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 13.548 A

USER

USER Estimated Free Energy of Binding = -6.65 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 13.36 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -8.14 kcal/mol

USER vdW + Hbond + desolv Energy = -7.87 kcal/mol

USER Electrostatic Energy = -0.27 kcal/mol

USER (2) Final Total Internal Energy = -1.89 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.89 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 16.993227 -4.246567 1.514207

USER NEWDPF axisangle0 -0.630970 -0.701480 0.331365 -75.196525

USER NEWDPF quaternion0 -0.384968 -0.427987 0.202173 -0.792308

USER NEWDPF dihe0 -153.06 -24.83 -9.13 176.54 -178.74

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 14.542 -8.820 0.461 -0.67 -0.00 +0.000 13.548

ATOM 2 C 0 15.644 -8.238 1.080 -0.49 -0.00 +0.000 13.548

ATOM 3 C 0 16.060 -6.964 0.712 -0.53 -0.00 +0.004 13.548

ATOM 4 C 0 15.366 -6.273 -0.282 -0.52 -0.02 +0.043 13.548

ATOM 5 C 0 14.259 -6.854 -0.905 -0.44 -0.00 +0.004 13.548

ATOM 6 C 0 13.853 -8.126 -0.531 -0.48 -0.00 +0.000 13.548

ATOM 7 C 0 15.783 -4.934 -0.688 -0.24 -0.05 +0.205 13.548

ATOM 8 N 0 16.803 -4.252 -0.292 -0.44 +0.03 -0.120 13.548

ATOM 9 N 0 16.784 -3.058 -0.997 -0.39 +0.04 -0.114 13.548

ATOM 10 C 0 15.740 -3.107 -1.750 -0.25 -0.06 +0.236 13.548

ATOM 11 O 0 15.050 -4.262 -1.613 -0.25 +0.06 -0.263 13.548

ATOM 12 S 0 15.159 -1.852 -2.819 -0.38 +0.01 -0.041 13.548

ATOM 13 C 0 15.618 -0.413 -1.863 -0.21 -0.02 +0.031 13.548

ATOM 14 C 0 16.614 0.405 -2.386 -0.19 -0.01 +0.008 13.548

ATOM 15 C 0 16.973 1.572 -1.720 -0.19 -0.03 +0.026 13.548

ATOM 16 C 0 16.347 1.889 -0.529 -0.18 -0.18 +0.111 13.548

ATOM 17 C 0 15.354 1.059 0.002 -0.26 -0.13 +0.108 13.548

ATOM 18 C 0 14.957 -0.097 -0.665 -0.29 -0.01 +0.008 13.548

ATOM 19 C 0 13.873 -0.954 -0.072 -0.37 -0.01 +0.034 13.548

ATOM 20 O 0 16.627 2.999 0.223 -0.11 +0.73 -0.357 13.548

ATOM 21 H 0 16.460 2.830 1.153 -0.43 -0.61 +0.218 13.548

ATOM 22 O 0 14.761 1.389 1.176 -0.21 +0.40 -0.357 13.548

ATOM 23 H 0 15.355 1.967 1.669 -0.34 -0.41 +0.218 13.548

TER

ENDMDL

MODEL 10

USER Run = 10

USER Cluster Rank = 2

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 51.592 A

USER

USER Estimated Free Energy of Binding = -6.13 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 32.13 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -7.62 kcal/mol

USER vdW + Hbond + desolv Energy = -7.52 kcal/mol

USER Electrostatic Energy = -0.10 kcal/mol

USER (2) Final Total Internal Energy = -1.87 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.87 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 17.190249 -21.266832 45.624592

USER NEWDPF axisangle0 0.885249 -0.436965 0.159363 74.668798

USER NEWDPF quaternion0 0.536873 -0.265004 0.096648 0.795110

USER NEWDPF dihe0 180.00 0.63 -63.65 27.01 -38.08

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 13.195 -20.205 48.933 -0.49 -0.00 +0.000 51.592

ATOM 2 C 0 14.072 -21.191 48.490 -0.27 -0.00 +0.000 51.592

ATOM 3 C 0 14.703 -21.062 47.259 -0.41 -0.00 +0.004 51.592

ATOM 4 C 0 14.451 -19.940 46.469 -0.48 -0.03 +0.043 51.592

ATOM 5 C 0 13.572 -18.948 46.911 -0.52 -0.00 +0.004 51.592

ATOM 6 C 0 12.947 -19.086 48.141 -0.63 -0.00 +0.000 51.592

ATOM 7 C 0 15.100 -19.780 45.171 -0.32 -0.11 +0.205 51.592

ATOM 8 N 0 14.626 -19.259 44.091 -0.36 +0.05 -0.120 51.592

ATOM 9 N 0 15.640 -19.308 43.146 -0.41 +0.04 -0.114 51.592

ATOM 10 C 0 16.641 -19.873 43.727 -0.28 -0.10 +0.236 51.592

ATOM 11 O 0 16.380 -20.204 45.012 -0.28 +0.15 -0.263 51.592

ATOM 12 S 0 18.184 -20.267 43.008 -0.45 +0.02 -0.041 51.592

ATOM 13 C 0 19.034 -20.891 44.452 -0.25 -0.01 +0.031 51.592

ATOM 14 C 0 18.457 -21.969 45.112 -0.26 -0.00 +0.008 51.592

ATOM 15 C 0 19.101 -22.538 46.206 -0.23 -0.01 +0.026 51.592

ATOM 16 C 0 20.300 -22.002 46.637 -0.19 -0.04 +0.111 51.592

ATOM 17 C 0 20.873 -20.909 45.979 -0.20 -0.03 +0.108 51.592

ATOM 18 C 0 20.261 -20.344 44.863 -0.28 -0.00 +0.008 51.592

ATOM 19 C 0 20.918 -19.181 44.172 -0.37 -0.01 +0.034 51.592

ATOM 20 O 0 21.015 -22.465 47.708 -0.12 +0.12 -0.357 51.592

ATOM 21 H 0 21.798 -21.928 47.852 -0.20 -0.12 +0.218 51.592

ATOM 22 O 0 22.047 -20.396 46.427 -0.09 +0.09 -0.357 51.592

ATOM 23 H 0 22.350 -20.928 47.172 -0.43 -0.11 +0.218 51.592

TER

ENDMDL

MODEL 6

USER Run = 6

USER Cluster Rank = 3

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 13.173 A

USER

USER Estimated Free Energy of Binding = -6.12 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 32.68 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -7.61 kcal/mol

USER vdW + Hbond + desolv Energy = -7.54 kcal/mol

USER Electrostatic Energy = -0.07 kcal/mol

USER (2) Final Total Internal Energy = -1.99 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.99 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 18.167684 -2.368128 -2.767414

USER NEWDPF axisangle0 0.909475 -0.358855 0.209949 -99.461393

USER NEWDPF quaternion0 0.693943 -0.273812 0.160195 -0.646381

USER NEWDPF dihe0 -156.15 23.31 -26.75 128.53 -177.90

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 15.513 -1.191 -7.194 -0.45 +0.00 +0.000 13.173

ATOM 2 C 0 16.686 -0.967 -6.479 -0.37 -0.00 +0.000 13.173

ATOM 3 C 0 16.729 -1.217 -5.113 -0.13 -0.00 +0.004 13.173

ATOM 4 C 0 15.589 -1.692 -4.463 -0.32 -0.01 +0.043 13.173

ATOM 5 C 0 14.411 -1.919 -5.178 -0.25 +0.00 +0.004 13.173

ATOM 6 C 0 14.378 -1.665 -6.541 -0.30 +0.00 +0.000 13.173

ATOM 7 C 0 15.608 -1.962 -3.029 -0.20 -0.06 +0.205 13.173

ATOM 8 N 0 16.554 -1.746 -2.180 -0.27 +0.05 -0.120 13.173

ATOM 9 N 0 16.073 -2.137 -0.938 -0.26 +0.05 -0.114 13.173

ATOM 10 C 0 14.879 -2.575 -1.141 -0.18 -0.07 +0.236 13.173

ATOM 11 O 0 14.509 -2.499 -2.440 -0.17 +0.06 -0.263 13.173

ATOM 12 S 0 13.800 -3.265 0.048 -0.53 +0.01 -0.041 13.173

ATOM 13 C 0 14.420 -4.942 0.072 -0.41 -0.01 +0.031 13.173

ATOM 14 C 0 15.355 -5.260 1.050 -0.57 -0.00 +0.008 13.173

ATOM 15 C 0 15.829 -6.562 1.159 -0.48 -0.01 +0.026 13.173

ATOM 16 C 0 15.378 -7.522 0.272 -0.58 -0.06 +0.111 13.173

ATOM 17 C 0 14.445 -7.198 -0.719 -0.41 -0.06 +0.108 13.173

ATOM 18 C 0 13.933 -5.907 -0.826 -0.39 -0.00 +0.008 13.173

ATOM 19 C 0 12.919 -5.603 -1.893 -0.33 -0.01 +0.034 13.173

ATOM 20 O 0 15.783 -8.829 0.271 -0.42 +0.34 -0.357 13.173

ATOM 21 H 0 15.693 -9.212 -0.605 -0.13 -0.31 +0.218 13.173

ATOM 22 O 0 14.024 -8.156 -1.583 -0.25 +0.42 -0.357 13.173

ATOM 23 H 0 14.131 -9.017 -1.162 -0.17 -0.39 +0.218 13.173

TER

ENDMDL

MODEL 8

USER Run = 8

USER Cluster Rank = 4

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 7.650 A

USER

USER Estimated Free Energy of Binding = -5.73 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 63.01 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -7.22 kcal/mol

USER vdW + Hbond + desolv Energy = -7.16 kcal/mol

USER Electrostatic Energy = -0.06 kcal/mol

USER (2) Final Total Internal Energy = -2.05 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -2.05 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 5.250501 -1.851383 -8.400252

USER NEWDPF axisangle0 0.135446 0.939784 -0.313783 -130.411094

USER NEWDPF quaternion0 0.122961 0.853153 -0.284857 -0.419364

USER NEWDPF dihe0 174.75 -29.64 -16.42 53.64 71.72

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 7.148 -3.175 -3.638 -0.57 +0.00 +0.000 7.650

ATOM 2 C 0 5.993 -3.036 -4.402 -0.48 +0.00 +0.000 7.650

ATOM 3 C 0 6.000 -2.237 -5.539 -0.40 +0.00 +0.004 7.650

ATOM 4 C 0 7.172 -1.574 -5.908 -0.39 +0.04 +0.043 7.650

ATOM 5 C 0 8.332 -1.713 -5.143 -0.29 +0.00 +0.004 7.650

ATOM 6 C 0 8.315 -2.512 -4.010 -0.55 +0.00 +0.000 7.650

ATOM 7 C 0 7.206 -0.728 -7.097 -0.21 +0.20 +0.205 7.650

ATOM 8 N 0 7.750 -0.966 -8.241 -0.28 -0.18 -0.120 7.650

ATOM 9 N 0 7.476 0.128 -9.049 -0.24 -0.09 -0.114 7.650

ATOM 10 C 0 6.804 0.949 -8.319 -0.20 +0.12 +0.236 7.650

ATOM 11 O 0 6.590 0.482 -7.068 -0.28 -0.12 -0.263 7.650

ATOM 12 S 0 6.236 2.537 -8.780 -0.14 -0.01 -0.041 7.650

ATOM 13 C 0 6.052 3.268 -7.159 -0.35 +0.00 +0.031 7.650

ATOM 14 C 0 7.010 4.196 -6.769 -0.30 -0.00 +0.008 7.650

ATOM 15 C 0 6.890 4.845 -5.545 -0.29 -0.01 +0.026 7.650

ATOM 16 C 0 5.824 4.536 -4.720 -0.30 -0.05 +0.111 7.650

ATOM 17 C 0 4.868 3.593 -5.108 -0.33 -0.03 +0.108 7.650

ATOM 18 C 0 4.952 2.955 -6.343 -0.52 -0.00 +0.008 7.650

ATOM 19 C 0 3.894 1.961 -6.733 -0.04 -0.00 +0.034 7.650

ATOM 20 O 0 5.610 5.095 -3.489 -0.23 +0.22 -0.357 7.650

ATOM 21 H 0 4.789 4.774 -3.108 -0.02 -0.16 +0.218 7.650

ATOM 22 O 0 3.836 3.302 -4.277 -0.44 +0.16 -0.357 7.650

ATOM 23 H 0 4.122 3.452 -3.368 -0.30 -0.16 +0.218 7.650

TER

ENDMDL

MODEL 3

USER Run = 3

USER Cluster Rank = 5

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 17.164 A

USER

USER Estimated Free Energy of Binding = -5.27 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 136.01 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -6.77 kcal/mol

USER vdW + Hbond + desolv Energy = -6.35 kcal/mol

USER Electrostatic Energy = -0.41 kcal/mol

USER (2) Final Total Internal Energy = -1.83 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.83 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 -0.300243 -18.126576 4.984325

USER NEWDPF axisangle0 -0.723647 0.178840 -0.666597 -92.685072

USER NEWDPF quaternion0 -0.523544 0.129387 -0.482270 -0.690345

USER NEWDPF dihe0 -156.76 -27.83 -120.34 -70.96 -1.83

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 -4.039 -14.378 4.994 -0.29 -0.00 +0.000 17.164

ATOM 2 C 0 -3.754 -15.699 5.327 -0.18 -0.00 +0.000 17.164

ATOM 3 C 0 -2.686 -16.355 4.726 -0.15 -0.00 +0.004 17.164

ATOM 4 C 0 -1.903 -15.682 3.787 -0.17 -0.01 +0.043 17.164

ATOM 5 C 0 -2.187 -14.356 3.452 -0.31 -0.00 +0.004 17.164

ATOM 6 C 0 -3.255 -13.710 4.056 -0.40 -0.00 +0.000 17.164

ATOM 7 C 0 -0.777 -16.349 3.141 -0.20 -0.05 +0.205 17.164

ATOM 8 N 0 0.049 -15.876 2.271 -0.38 +0.03 -0.120 17.164

ATOM 9 N 0 0.959 -16.885 1.995 -0.45 +0.02 -0.114 17.164

ATOM 10 C 0 0.598 -17.895 2.709 -0.12 -0.06 +0.236 17.164

ATOM 11 O 0 -0.494 -17.637 3.463 -0.11 +0.07 -0.263 17.164

ATOM 12 S 0 1.332 -19.480 2.728 -0.15 +0.01 -0.041 17.164

ATOM 13 C 0 2.765 -19.132 3.739 -0.20 -0.01 +0.031 17.164

ATOM 14 C 0 2.897 -17.838 4.228 -0.38 -0.00 +0.008 17.164

ATOM 15 C 0 3.957 -17.519 5.070 -0.32 -0.01 +0.026 17.164

ATOM 16 C 0 4.882 -18.496 5.389 -0.25 -0.04 +0.111 17.164

ATOM 17 C 0 4.755 -19.794 4.886 -0.31 -0.05 +0.108 17.164

ATOM 18 C 0 3.683 -20.143 4.067 -0.22 -0.00 +0.008 17.164

ATOM 19 C 0 3.571 -21.554 3.562 -0.14 -0.01 +0.034 17.164

ATOM 20 O 0 5.973 -18.298 6.192 -0.81 +0.12 -0.357 17.164

ATOM 21 H 0 6.668 -18.926 5.982 -0.37 -0.26 +0.218 17.164

ATOM 22 O 0 5.680 -20.733 5.208 -0.18 +0.30 -0.357 17.164

ATOM 23 H 0 6.513 -20.288 5.407 -0.25 -0.45 +0.218 17.164

TER

ENDMDL

MODEL 4

USER Run = 4

USER Cluster Rank = 6

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 41.476 A

USER

USER Estimated Free Energy of Binding = -5.03 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 205.60 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -6.52 kcal/mol

USER vdW + Hbond + desolv Energy = -6.56 kcal/mol

USER Electrostatic Energy = +0.04 kcal/mol

USER (2) Final Total Internal Energy = -1.92 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.92 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 9.224051 23.518576 33.393671

USER NEWDPF axisangle0 0.401535 -0.899572 -0.171870 -76.924302

USER NEWDPF quaternion0 0.249754 -0.559532 -0.106903 -0.783019

USER NEWDPF dihe0 -161.01 19.69 -1.93 123.92 -122.20

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 8.029 24.041 28.262 -0.54 -0.00 +0.000 41.476

ATOM 2 C 0 8.926 23.483 29.169 -0.48 -0.00 +0.000 41.476

ATOM 3 C 0 9.028 23.998 30.456 -0.37 -0.00 +0.004 41.476

ATOM 4 C 0 8.228 25.077 30.833 -0.22 -0.01 +0.043 41.476

ATOM 5 C 0 7.327 25.638 29.925 -0.22 +0.00 +0.004 41.476

ATOM 6 C 0 7.233 25.119 28.643 -0.38 +0.00 +0.000 41.476

ATOM 7 C 0 8.316 25.636 32.178 -0.09 -0.02 +0.205 41.476

ATOM 8 N 0 9.334 26.165 32.766 -0.12 +0.01 -0.120 41.476

ATOM 9 N 0 8.902 26.579 34.017 -0.10 +0.01 -0.114 41.476

ATOM 10 C 0 7.659 26.249 34.091 -0.06 -0.01 +0.236 41.476

ATOM 11 O 0 7.211 25.646 32.967 -0.07 -0.00 -0.263 41.476

ATOM 12 S 0 6.600 26.458 35.466 -0.16 +0.00 -0.041 41.476

ATOM 13 C 0 6.946 24.938 36.341 -0.28 -0.00 +0.031 41.476

ATOM 14 C 0 7.461 25.049 37.628 -0.41 -0.00 +0.008 41.476

ATOM 15 C 0 7.694 23.905 38.383 -0.52 -0.01 +0.026 41.476

ATOM 16 C 0 7.431 22.666 37.829 -0.56 -0.03 +0.111 41.476

ATOM 17 C 0 6.925 22.555 36.530 -0.13 -0.01 +0.108 41.476

ATOM 18 C 0 6.654 23.689 35.768 -0.33 -0.00 +0.008 41.476

ATOM 19 C 0 6.094 23.529 34.382 -0.29 +0.00 +0.034 41.476

ATOM 20 O 0 7.636 21.472 38.467 -0.51 +0.15 -0.357 41.476

ATOM 21 H 0 7.711 20.756 37.832 -0.28 -0.08 +0.218 41.476

ATOM 22 O 0 6.683 21.327 36.006 -0.14 +0.09 -0.357 41.476

ATOM 23 H 0 6.587 20.697 36.730 -0.32 -0.05 +0.218 41.476

TER

ENDMDL

MODEL 5

USER Run = 5

USER Cluster Rank = 7

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 23.519 A

USER

USER Estimated Free Energy of Binding = -4.47 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 527.92 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -5.96 kcal/mol

USER vdW + Hbond + desolv Energy = -5.96 kcal/mol

USER Electrostatic Energy = -0.00 kcal/mol

USER (2) Final Total Internal Energy = -2.10 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -2.10 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 24.432332 -0.108659 0.228783

USER NEWDPF axisangle0 0.264772 0.884267 0.384665 -75.329619

USER NEWDPF quaternion0 0.161787 0.540323 0.235046 -0.791599

USER NEWDPF dihe0 -169.70 20.59 -17.81 35.77 -97.90

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 23.057 -4.483 2.875 -0.31 -0.00 +0.000 23.519

ATOM 2 C 0 23.055 -3.861 1.630 -0.23 -0.00 +0.000 23.519

ATOM 3 C 0 23.185 -2.480 1.540 -0.18 -0.00 +0.004 23.519

ATOM 4 C 0 23.317 -1.723 2.705 -0.23 -0.01 +0.043 23.519

ATOM 5 C 0 23.320 -2.345 3.955 -0.26 -0.00 +0.004 23.519

ATOM 6 C 0 23.189 -3.723 4.034 -0.38 -0.00 +0.000 23.519

ATOM 7 C 0 23.455 -0.271 2.638 -0.15 -0.06 +0.205 23.519

ATOM 8 N 0 22.530 0.624 2.558 -0.47 +0.06 -0.120 23.519

ATOM 9 N 0 23.167 1.856 2.560 -0.54 +0.06 -0.114 23.519

ATOM 10 C 0 24.428 1.605 2.623 -0.08 -0.08 +0.236 23.519

ATOM 11 O 0 24.696 0.280 2.675 -0.19 +0.06 -0.263 23.519

ATOM 12 S 0 25.731 2.770 2.590 -0.43 +0.01 -0.041 23.519

ATOM 13 C 0 27.127 1.653 2.570 -0.22 -0.00 +0.031 23.519

ATOM 14 C 0 27.786 1.482 1.358 -0.16 -0.00 +0.008 23.519

ATOM 15 C 0 28.916 0.673 1.291 -0.12 -0.00 +0.026 23.519

ATOM 16 C 0 29.353 0.029 2.433 -0.11 +0.01 +0.111 23.519

ATOM 17 C 0 28.681 0.192 3.649 -0.16 +0.03 +0.108 23.519

ATOM 18 C 0 27.567 1.022 3.745 -0.25 +0.00 +0.008 23.519

ATOM 19 C 0 26.883 1.185 5.074 -0.30 +0.00 +0.034 23.519

ATOM 20 O 0 30.439 -0.803 2.486 -0.05 -0.04 -0.357 23.519

ATOM 21 H 0 30.453 -1.291 3.313 -0.47 +0.05 +0.218 23.519

ATOM 22 O 0 29.126 -0.458 4.754 -0.37 -0.24 -0.357 23.519

ATOM 23 H 0 30.056 -0.681 4.626 -0.29 +0.16 +0.218 23.519

TER

ENDMDL

MODEL 2

USER Run = 2

USER Cluster Rank = 8

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 31.022 A

USER

USER Estimated Free Energy of Binding = -4.44 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 557.85 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -5.93 kcal/mol

USER vdW + Hbond + desolv Energy = -5.79 kcal/mol

USER Electrostatic Energy = -0.14 kcal/mol

USER (2) Final Total Internal Energy = -2.04 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -2.04 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 25.963658 -18.587115 11.814539

USER NEWDPF axisangle0 -0.275019 0.873225 0.402296 -52.327089

USER NEWDPF quaternion0 -0.121265 0.385035 0.177386 -0.897539

USER NEWDPF dihe0 -153.97 21.32 -50.82 67.26 -161.40

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 23.481 -21.647 15.351 -0.23 -0.00 +0.000 31.022

ATOM 2 C 0 24.071 -21.616 14.091 -0.22 -0.00 +0.000 31.022

ATOM 3 C 0 24.234 -20.407 13.426 -0.15 -0.00 +0.004 31.022

ATOM 4 C 0 23.802 -19.225 14.028 -0.28 -0.00 +0.043 31.022

ATOM 5 C 0 23.210 -19.253 15.293 -0.22 +0.00 +0.004 31.022

ATOM 6 C 0 23.051 -20.464 15.948 -0.26 -0.00 +0.000 31.022

ATOM 7 C 0 23.961 -17.942 13.351 -0.21 +0.01 +0.205 31.022

ATOM 8 N 0 24.121 -17.709 12.093 -0.76 -0.02 -0.120 31.022

ATOM 9 N 0 24.186 -16.331 11.948 -0.32 -0.04 -0.114 31.022

ATOM 10 C 0 24.079 -15.843 13.135 -0.24 +0.04 +0.236 31.022

ATOM 11 O 0 23.933 -16.797 14.081 -0.21 -0.04 -0.263 31.022

ATOM 12 S 0 24.158 -14.156 13.585 -0.65 -0.01 -0.041 31.022

ATOM 13 C 0 25.006 -14.306 15.152 -0.26 +0.00 +0.031 31.022

ATOM 14 C 0 26.349 -14.663 15.115 -0.16 +0.00 +0.008 31.022

ATOM 15 C 0 27.080 -14.737 16.296 -0.11 +0.00 +0.026 31.022

ATOM 16 C 0 26.447 -14.478 17.498 -0.12 +0.04 +0.111 31.022

ATOM 17 C 0 25.093 -14.132 17.534 -0.18 +0.06 +0.108 31.022

ATOM 18 C 0 24.351 -14.020 16.361 -0.30 +0.00 +0.008 31.022

ATOM 19 C 0 22.902 -13.628 16.440 -0.30 +0.01 +0.034 31.022

ATOM 20 O 0 27.056 -14.536 18.723 -0.03 -0.13 -0.357 31.022

ATOM 21 H 0 26.421 -14.758 19.407 +0.04 +0.14 +0.218 31.022

ATOM 22 O 0 24.493 -13.890 18.727 -0.61 -0.40 -0.357 31.022

ATOM 23 H 0 25.171 -13.645 19.368 -0.02 +0.18 +0.218 31.022

TER

ENDMDL

MODEL 1

USER Run = 1

USER Cluster Rank = 9

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 25.438 A

USER

USER Estimated Free Energy of Binding = -4.38 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 619.49 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -5.87 kcal/mol

USER vdW + Hbond + desolv Energy = -5.85 kcal/mol

USER Electrostatic Energy = -0.01 kcal/mol

USER (2) Final Total Internal Energy = -2.00 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -2.00 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 -3.861535 -1.265298 22.080385

USER NEWDPF axisangle0 -0.969966 0.046522 0.238750 158.853185

USER NEWDPF quaternion0 -0.953497 0.045732 0.234697 0.183495

USER NEWDPF dihe0 -159.85 23.67 160.55 108.47 94.13

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 -8.033 1.577 23.677 -0.07 -0.00 +0.000 25.438

ATOM 2 C 0 -6.661 1.604 23.446 -0.14 -0.00 +0.000 25.438

ATOM 3 C 0 -5.936 0.420 23.405 -0.23 +0.00 +0.004 25.438

ATOM 4 C 0 -6.592 -0.797 23.598 -0.21 +0.01 +0.043 25.438

ATOM 5 C 0 -7.969 -0.827 23.830 -0.18 -0.00 +0.004 25.438

ATOM 6 C 0 -8.684 0.360 23.870 -0.18 -0.00 +0.000 25.438

ATOM 7 C 0 -5.854 -2.055 23.561 -0.08 +0.10 +0.205 25.438

ATOM 8 N 0 -5.511 -2.759 22.537 -0.37 -0.11 -0.120 25.438

ATOM 9 N 0 -4.794 -3.844 23.020 -0.71 -0.09 -0.114 25.438

ATOM 10 C 0 -4.777 -3.717 24.301 -0.14 +0.06 +0.236 25.438

ATOM 11 O 0 -5.427 -2.610 24.725 -0.26 -0.02 -0.263 25.438

ATOM 12 S 0 -4.073 -4.826 25.455 -0.50 +0.01 -0.041 25.438

ATOM 13 C 0 -5.560 -5.628 26.040 -0.39 -0.01 +0.031 25.438

ATOM 14 C 0 -6.342 -4.930 26.952 -0.47 -0.00 +0.008 25.438

ATOM 15 C 0 -7.541 -5.475 27.399 -0.31 -0.01 +0.026 25.438

ATOM 16 C 0 -7.926 -6.722 26.943 -0.37 -0.03 +0.111 25.438

ATOM 17 C 0 -7.132 -7.429 26.035 -0.16 -0.01 +0.108 25.438

ATOM 18 C 0 -5.944 -6.888 25.550 -0.29 -0.00 +0.008 25.438

ATOM 19 C 0 -5.127 -7.671 24.560 -0.22 -0.01 +0.034 25.438

ATOM 20 O 0 -9.073 -7.365 27.323 -0.13 +0.17 -0.357 25.438

ATOM 21 H 0 -8.992 -8.312 27.186 +0.05 -0.05 +0.218 25.438

ATOM 22 O 0 -7.529 -8.655 25.608 -0.56 +0.02 -0.357 25.438

ATOM 23 H 0 -8.489 -8.711 25.686 +0.06 -0.03 +0.218 25.438

TER

ENDMDL

MODEL 9

USER Run = 9

USER Cluster Rank = 10

USER Number of conformations in this cluster = 1

USER

USER RMSD from reference structure = 19.686 A

USER

USER Estimated Free Energy of Binding = -4.12 kcal/mol [=(1)+(2)+(3)-(4)]

USER Estimated Inhibition Constant, Ki = 951.19 uM (micromolar) [Temperature = 298.15 K]

USER

USER (1) Final Intermolecular Energy = -5.61 kcal/mol

USER vdW + Hbond + desolv Energy = -5.47 kcal/mol

USER Electrostatic Energy = -0.14 kcal/mol

USER (2) Final Total Internal Energy = -1.86 kcal/mol

USER (3) Torsional Free Energy = +1.49 kcal/mol

USER (4) Unbound System's Energy [=(2)] = -1.86 kcal/mol

USER

USER

USER

USER DPF = C:/Users/A/Desktop/docking/dock.dpf

USER NEWDPF move lig.pdbqt

USER NEWDPF about 0.195300 -0.322700 0.046500

USER NEWDPF tran0 0.328951 16.840606 9.246315

USER NEWDPF axisangle0 -0.703474 -0.050404 -0.708931 87.815856

USER NEWDPF quaternion0 -0.487860 -0.034955 -0.491645 0.720455

USER NEWDPF dihe0 -170.18 -22.48 -178.68 -176.42 -119.44

USER

USER x y z vdW Elec q RMS

ATOM 1 C 0 -0.965 13.345 5.487 -0.37 -0.00 +0.000 19.686

ATOM 2 C 0 -0.457 14.618 5.728 -0.30 -0.00 +0.000 19.686

ATOM 3 C 0 -0.698 15.246 6.943 -0.22 -0.00 +0.004 19.686

ATOM 4 C 0 -1.452 14.594 7.919 -0.17 -0.01 +0.043 19.686

ATOM 5 C 0 -1.963 13.317 7.680 -0.23 -0.00 +0.004 19.686

ATOM 6 C 0 -1.718 12.698 6.464 -0.24 -0.00 +0.000 19.686

ATOM 7 C 0 -1.720 15.233 9.204 -0.08 -0.06 +0.205 19.686

ATOM 8 N 0 -2.381 16.314 9.445 -0.05 +0.04 -0.120 19.686

ATOM 9 N 0 -2.385 16.480 10.822 -0.07 +0.06 -0.114 19.686

ATOM 10 C 0 -1.709 15.494 11.302 -0.09 -0.12 +0.236 19.686

ATOM 11 O 0 -1.253 14.658 10.342 -0.11 +0.08 -0.263 19.686

ATOM 12 S 0 -1.319 15.210 12.982 -0.44 +0.03 -0.041 19.686

ATOM 13 C 0 -1.332 16.895 13.578 -0.29 -0.03 +0.031 19.686

ATOM 14 C 0 -0.482 17.798 12.950 -0.23 -0.01 +0.008 19.686

ATOM 15 C 0 -0.490 19.136 13.328 -0.23 -0.03 +0.026 19.686

ATOM 16 C 0 -1.331 19.545 14.346 -0.26 -0.11 +0.111 19.686

ATOM 17 C 0 -2.176 18.633 14.986 -0.24 -0.10 +0.108 19.686

ATOM 18 C 0 -2.208 17.295 14.602 -0.29 -0.01 +0.008 19.686

ATOM 19 C 0 -3.144 16.349 15.301 -0.33 -0.04 +0.034 19.686

ATOM 20 O 0 -1.414 20.828 14.815 -0.18 +0.32 -0.357 19.686

ATOM 21 H 0 -1.912 20.859 15.635 -0.45 -0.24 +0.218 19.686

ATOM 22 O 0 -2.987 19.058 15.988 -0.19 +0.31 -0.357 19.686

ATOM 23 H 0 -2.632 19.882 16.341 -0.41 -0.23 +0.218 19.686

TER

ENDMDL

AVSFLD: # AVS field file

AVSFLD: #

AVSFLD: # Created by AutoDock

AVSFLD: #

AVSFLD: ndim=2 # number of dimensions in the field

AVSFLD: nspace=1 # number of physical coordinates

AVSFLD: veclen=7 # vector size

AVSFLD: dim1=23 # atoms

AVSFLD: dim2=10 # conformations

AVSFLD: data=Real # data type (byte,integer,Real,double)

AVSFLD: field=uniform # field coordinate layout

AVSFLD: label= x y z vdW Elec q RMS

AVSFLD: variable 1 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 5 stride = 12

AVSFLD: variable 2 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 6 stride = 12

AVSFLD: variable 3 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 7 stride = 12

AVSFLD: variable 4 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 8 stride = 12

AVSFLD: variable 5 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 9 stride = 12

AVSFLD: variable 6 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 10 stride = 12

AVSFLD: variable 7 file = C:/Users/A/Desktop/docking/dock.dlg.pdb filetype = ascii offset = 11 stride = 12

AVSFLD: # end of file

|  |
| --- |
|  |
| a) |
|  |
|  |
| b) |
| **Figure S1.** Correlation between calculated and experimental bond lengths **(a)** and bond angles **(b)**  at B3LYP/6-311++G(d,p) and M062X/6-311++G(d,p). |

**Figure S2.** Graphical correlation between the experimental and calculated Infrared wavenumbers of 4-(5-Phenyl-1,3,4-oxadiazol-2-ylthio)-3-methylbenzene-1,2diol (POTMBD): a) at B3LY/6-311++G(d,p) level (black), scaled by 0.920; b) at M06/6-311++G(d,p) level, scaled by 0.909.