Supporting Information for "Automatic Screen-out of Ir(III) Complex emitters by Combined Machine Learning and Computational Analysis"

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Computational details

Starting from the optimized ground state (GS) structure via the aforementioned semi-empirical method, we re-optimize the GS structure via density functional theory (DFT) with B3LYP functional. The T_1 state is optimized via unrestricted DFT with the same functional and basis set. Time-dependent DFT (TDDFT) with PBE0-1/3 functional within the Tamm-Dancoff approximation (TDA) is performed at the T_1 optimized geometry to obtain the excitation energy. All geometry optimizations and excitation energy calculations are carried out with the 6-31G** basis set (LANDL2DZ basis and corresponding effective core potential for Ir atom) in Gaussian16 quantum chemistry package.[1] The spin-orbit coupling (SOC) between T_1 and S_0 is evaluated via TDDFT with B3LYP functional and DKH-def2-TZVP basis set, and the transition dipole moment (TDM) of T_1 is then calculated via the sum-over-state (SOS) method[2] with twenty-five singlets and twenty-five triplets. The SOC and TDM calculations of T_1 are carried out in ORCA quantum chemistry package.[3,4] The radiative and non-radiative decay rate constants are evaluated with thermal vibration correlation function (TVCF) method in molecular property prediction package MOMAP.[5–7]

Supplementary figures

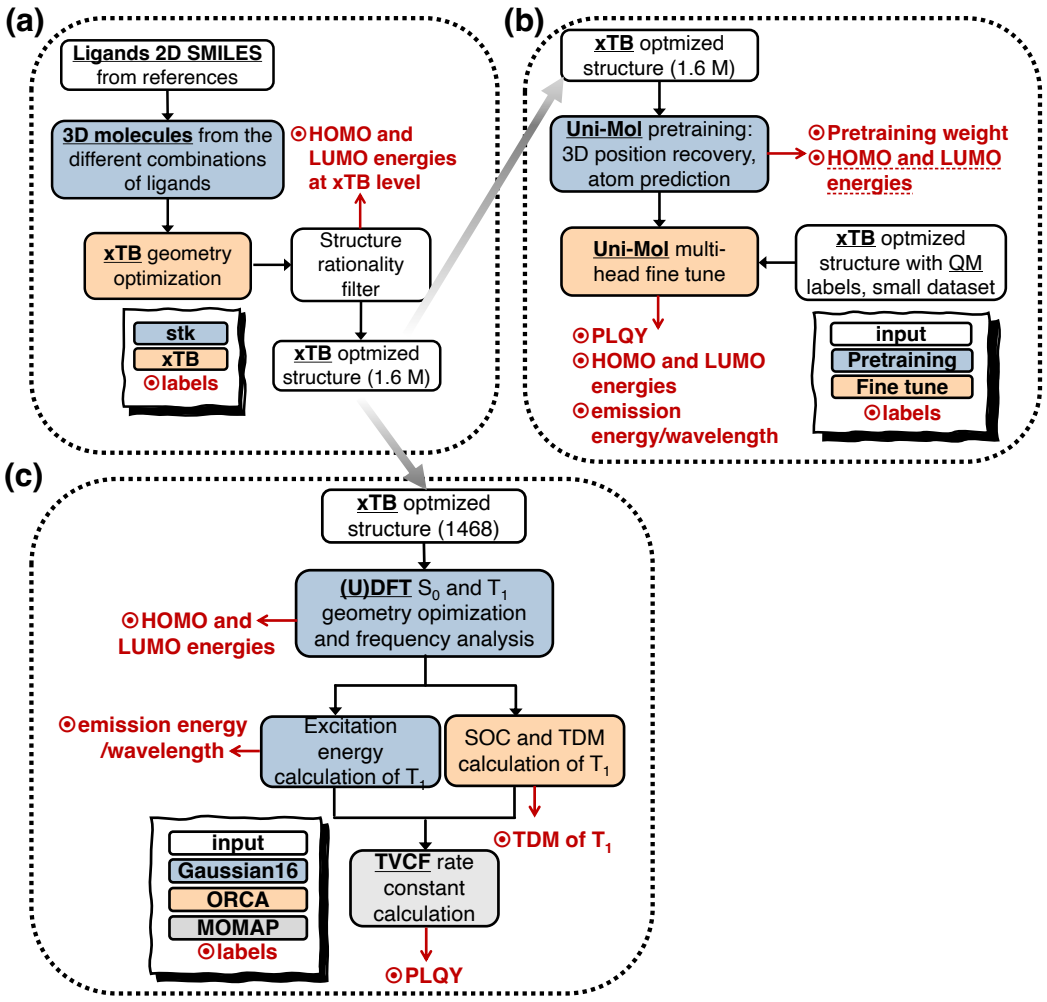

Figure S1: Workflows involved in this work. (a) Automatic construction of reasonable initial structures of the candidates pool. (b) Uni-Mol training process. (c) QM calculation process for selected candidates.

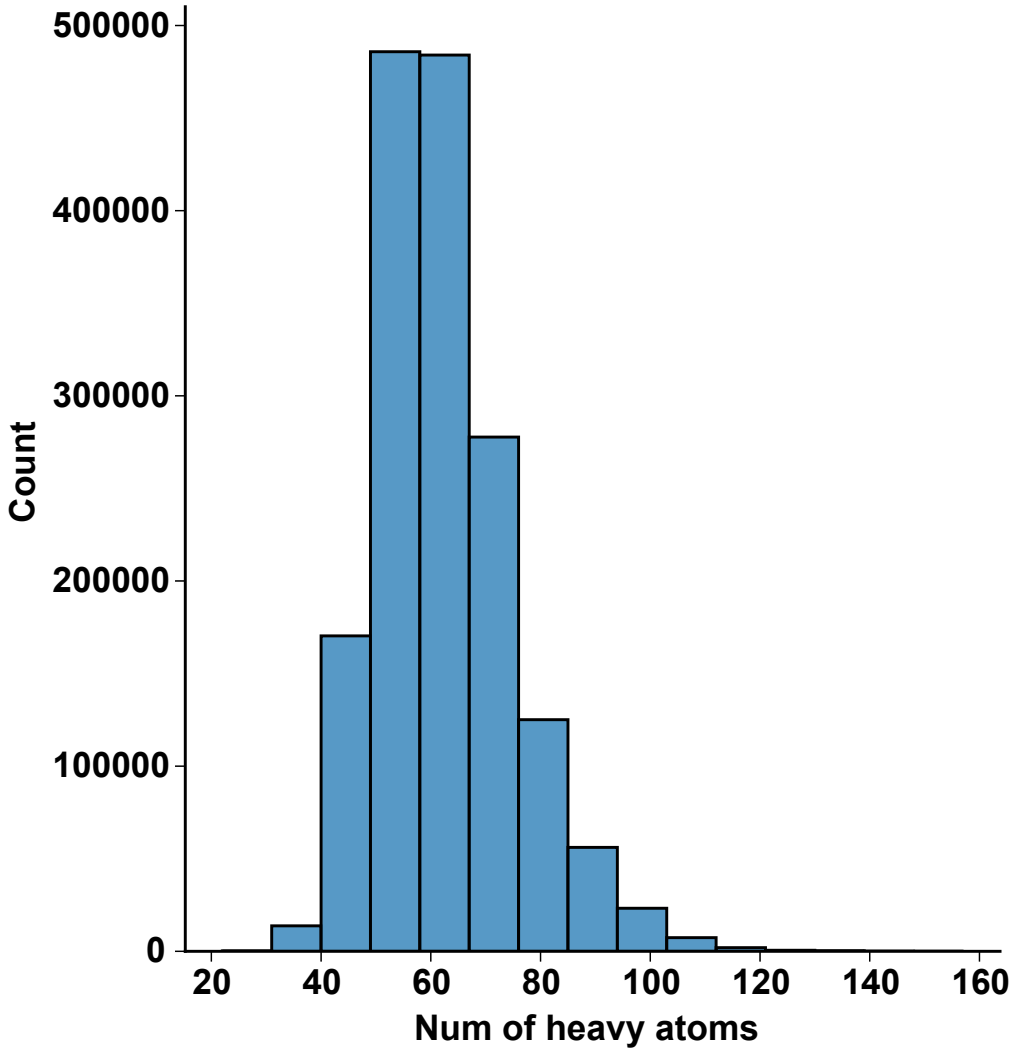

Figure S2: The distribution of heavy atoms of all the structures in candidates pool.

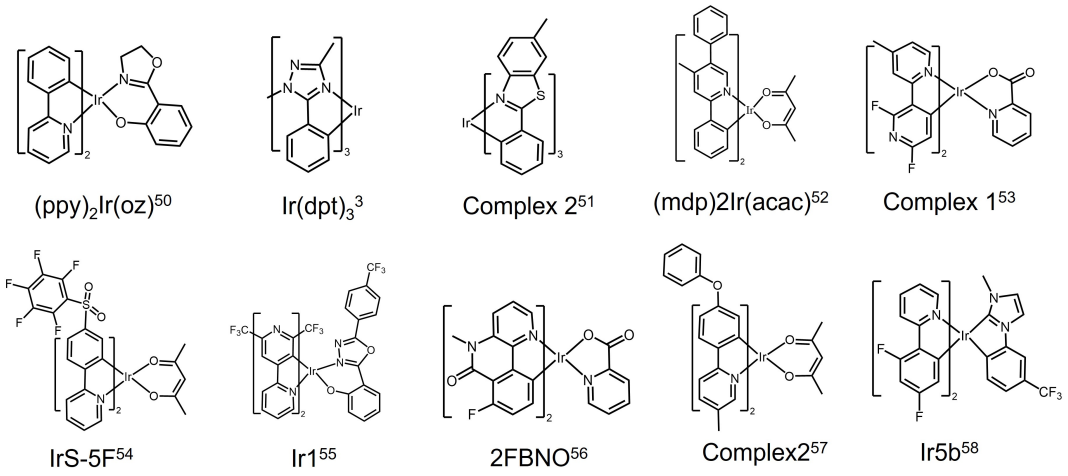

Figure S3: The configurations of molecules in the Table 1 of the main text.

3D coordinates of the five screened-out candidates that shown in Figure 5 of the main text

89_89_228

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C 2.734194 3.167841 -0.075772

H 6.414117 1.478053 0.760935

H 6.510301 1.809214 -0.978723

H 7.364154 2.834044 0.168237

H 5.102101 3.030355 2.274781

H 4.407868 4.519010 1.632748

H 6.157621 4.329470 1.714703

H 6.334727 4.819145 -0.800053

H 4.588229 5.035255 -0.852047

H 5.362825 3.880934 -1.936209

H 4.712889 0.467638 -0.386879

H 2.532465 -0.554121 -0.679624

H -3.058844 2.276267 -0.542866

H 2.740364 4.229234 0.095861

C 1.182309 -6.702633 -0.705057

C 1.080733 -5.776309 -1.919478

C 2.414339 -5.819875 -2.679279

C -0.050836 -6.281889 -2.825228

C 0.793230 -4.340556 -1.526785

C 0.650801 -3.916104 -0.208392

C 0.387214 -2.584129 0.047359

N 0.269981 -1.663726 -0.898938

C 0.419594 -2.036764 -2.186095

C 0.288061 -0.952399 -3.159821

C -0.140368 0.309196 -2.662017

C -0.276862 1.334118 -3.600406

C 0.001434 1.077314 -4.926869

F -0.139337 2.044982 -5.845026

N 0.420713 -0.081107 -5.392046

C 0.558676 -1.051302 -4.522355

F 1.018472 -2.196700 -5.071804

C 0.667367 -3.367645 -2.511982

H 1.989420 -6.396028 -0.043348

H 0.249220 -6.721068 -0.146145

H 1.391932 -7.715773 -1.040352

H 3.220724 -5.447703 -2.050069

H 2.377812 -5.216181 -3.581736

H 2.644952 -6.843769 -2.963782

H 0.130684 -7.318303 -3.099734

H -0.121048 -5.697379 -3.738137

H -1.005924 -6.225354 -2.306441

H 0.736194 -4.595217 0.622253

H 0.270970 -2.236095 1.065350

H -0.597697 2.322222 -3.308966

H 0.760638 -3.649067 -3.544931

C 1.017959 0.549771 4.874377

C 0.002294 0.239319 3.817558

C 0.288835 0.476466 2.477252

C -0.608111 0.195069 1.453558

C -1.855344 -0.350341 1.843378

C -2.728189 -0.602960 0.725718

N -2.279595 -0.369893 -0.521665

C -3.316160 -0.680191 -1.338538

C -3.298157 -0.567619 -2.814269

N -4.360403 -1.088763 -0.661084

N -3.994616 -1.040299 0.632270

C -4.951239 -1.391882 1.640076

C -2.159037 -0.602700 3.180104

H -3.107357 -1.028641 3.468614

C -1.230095 -0.308387 4.156749

H 0.546324 0.666040 5.847337

H 1.744544 -0.261244 4.943888

H 1.558636 1.462258 4.631518

H 1.255697 0.903308 2.238445

H -2.962073 0.425183 -3.104712

H -4.297077 -0.751226 -3.198094

H -2.608496 -1.293983 -3.240907

H -5.097501 -0.563316 2.334518

H -5.887157 -1.604663 1.126653

H -4.631466 -2.279897 2.188068

H -1.464531 -0.500815 5.194090

All ligands 2D SMILES collected from experimental publications

All the Smiles below are 278 bidentate ligands collected from experimental publications that report the Ir(III) complex phosphors

0 c1ccc(Oc2ccc(-c3ccccn3)cc2)cc1

1 c1ccc(Sc2ccc(-c3ccccn3)cc2)cc1

2 O=S(=O)(c1ccccc1)c1ccc(-c2ccccn2)cc1

3 c1ccc(N(c2ccccc2)c2ccc(-c3ccccn3)cc2)cc1

4 O=P(c1ccccc1)(c1ccccc1)c1ccc(-c2ccccn2)cc1

5 c1ccc([Si](c2ccccc2)(c2ccccc2)c2ccc(-c3ccccn3)cc2)cc1

6 c1ccc([Ge](c2ccccc2)(c2ccccc2)c2ccc(-c3ccccn3)cc2)cc1

7 c1ccc(-c2ccc(-n3c4ccccc4c4ccccc43)cc2)nc1

8 c1ccc(-c2nnc(-c3ccc(-c4ccccn4)cc3)o2)cc1

9 CC(C)(C)c1ccc(-c2nnc(-c3ccc(-c4ccccn4)cc3)o2)cc1

10 c1ccc(N(c2ccccc2)c2ccccc2-c2cccc(-c3ncccc3N(c3ccccc3)c3ccccc3)c2)cc1

11 c1ccc(N(c2ccccc2)c2ccc(-c3cccc(-c4ccc(N(c5ccccc5)c5ccccc5)cn4)c3)cc2)cc1

12 CCC1(CC)c2cc(-c3ccccn3)ccc2-c2ccc(N(c3ccc(OC)cc3)c3ccc(OC)cc3)cc21

13 Cc1ccc(C2(c3ccccc3)c3ccccc3-c3ccc(-c4ccccn4)cc32)cc1

14 Cc1ccc(C2(c3ccc(C)cc3)c3ccccc3-c3ccc(-c4ccccn4)cc32)cc1

15 c1ccc(-c2ccc(-c3ccccc3)nn2)cc1

16 c1ccc(-c2ccc(-n3c4ccccc4c4ccccc43)nn2)cc1

17 c1ccc(-c2ccc(N(c3ccccc3)c3ccccc3)nn2)cc1

18 Cc1ccc(-c2ccc(F)c(F)c2)nn1

19 c1ccc(-c2nc3ccccc3s2)cc1

20 Fc1ccc2nc(-c3ccccc3)sc2c1

21 Cc1ccc2nc(-c3ccccc3)sc2c1

22 COc1ccc2nc(-c3ccccc3)sc2c1

23 Fc1ccc(-c2nccs2)cc1

24 Fc1ccc(-c2nccs2)c(F)c1

25 Cn1c(-c2ccccc2)nc2ccccc21

26 Cn1c(-c2ccc(N(c3ccccc3)c3ccccc3)cc2)nc2ccccc21

27 Cn1c(-c2ccc(N(c3ccc(N(c4ccccc4)c4ccccc4)cc3)c3ccc(N(c4ccccc4)c4ccccc4)cc3)cc2)nc2ccccc21

28 Cn1c(-c2ccc(N(c3ccc(-n4c5ccccc5c5ccccc54)cc3)c3ccc(-n4c5ccccc5c5ccccc54)cc3)cc2)nc2ccccc21

29 Cn1c(-c2ccc(N(c3ccc(P(=O)(c4ccccc4)c4ccccc4)cc3)c3ccc(P(=O)(c4ccccc4)c4ccccc4)cc3)cc2)nc2ccc

30 Cn1c(=O)c2c(C(F)(F)F)cccc2c2ncccc21

31 CC(=O)CC(C)=O

32 CCC1(CC)c2ccccc2-c2cc(-c3nc4ccccc4n3-c3ccccc3)ccc21

33 O=S(=O)(c1ccc(F)cc1)c1ccc(-c2ccccn2)cc1

34 O=S(=O)(c1ccc(-c2ccccn2)cc1)c1ccc(F)cc1F

35 O=S(=O)(c1ccc(-c2ccccn2)cc1)c1cc(F)c(F)c(F)c1

36 O=S(=O)(c1ccc(-c2ccccn2)cc1)c1c(F)c(F)c(F)c(F)c1F

37 Cc1ccc(-c2ccc(Oc3ccccc3)cc2)nc1

38 Fc1ccc(C2NC=CS2)c(F)c1

39 CC(C)c1cc(-c2ccc(-c3nc4ccccc4s3)cc2)cc(C(C)C)c1

40 c1ccc(-c2nc3ccccn3c2-c2ccccc2)cc1

41 Cc1ccc2nc(-c3ccccc3)c(C)n2c1

42 Cc1c(-c2ccccc2)nc2ccccn12

43 Cc1ccc(-c2cn3ccccc3n2)cc1

44 Fc1ccc(-c2cn3ccccc3n2)cc1

45 Cc1ccc(-c2cn3cc(C)ccc3n2)cc1

46 FC(F)(F)c1ccc(-c2ccccc2)nc1

47 Cc1ccc(-c2ccc(C(F)(F)F)cn2)cc1

48 FC(F)(F)c1ccc(-c2ccc(Oc3ccccc3)cc2)nc1

49 O=S(=O)(c1ccccc1)c1ccc(-c2ccc(C(F)(F)F)cn2)cc1

50 FC(F)(F)c1ccc(-c2ccc(N(c3ccccc3)c3ccccc3)cc2)nc1

51 CC(C)(C)C(=O)CC(=O)C(C)(C)C

52 c1ccc(-c2ccccn2)cc1

53 CC(C)(C)C(=O)CC(=O)Cn1c2ccccc2c2ccccc21

54 Cc1cc(C)cc(-c2cc(C)ccn2)c1

55 Cc1cc(C)cc(-c2cc(C(F)(F)F)ccn2)c1

56 CCCc1ccnc(-c2cc(C)cc(C)c2)c1

57 Cc1cc(C)cc(-c2cc(-c3ccccc3)ccn2)c1

58 FC(F)(F)c1ccc(-c2ccccn2)cc1

59 O=P(NP(=O)(c1ccccc1)c1ccccc1)(c1ccccc1)c1ccccc1

60 O=P(NP(=O)(c1ccc(C(F)(F)F)cc1)c1ccc(C(F)(F)F)cc1)(c1ccc(C(F)(F)F)cc1)c1ccc(C(F)(F)F)cc1

61 FC(F)(F)c1ccccc1-c1ccccn1

62 FC(F)(F)c1cccc(-c2ccccn2)c1

63 FC(F)(F)c1cc(-c2ccccn2)cc(C(F)(F)F)c1

64 FC(F)(F)c1ccc(-c2ccccn2)c(C(F)(F)F)c1

65 FC(F)(F)c1cc(-c2ccccn2)cc(C(F)(F)F)n1

66 FC(F)(F)c1ccc(-c2ccccn2)c(C(F)(F)F)n1

67 Fc1cnc(-c2ccc(C(F)(F)F)cc2)nc1

68 Fc1cnc(-c2ccc(F)cc2F)nc1

69 FC(F)(F)c1ccc2nc(-c3ccccc3)sc2c1

70 Fc1cc(F)c2sc(-c3ccccc3)nc2c1

71 Cc1nn(-c2ccccc2Cl)c(O)c1C=O

72 Fc1cc(F)c(-c2ccccn2)cc1F

73 Oc1ccccc1-c1nnc(-c2ccccc2)o1

74 Oc1ccccc1-c1nnc(-c2ccc(F)cc2)o1

75 Oc1ccccc1-c1nnc(-c2ccc(C(F)(F)F)cc2)o1

76 Oc1ccccc1-c1nnc(-c2cc(C(F)(F)F)cc(C(F)(F)F)c2)o1

77 Oc1ccccc1-c1nnc(-c2cc(F)c(F)c(F)c2F)o1

78 Oc1ccccc1-c1nnc(-c2c(F)c(F)c(F)c(F)c2F)o1

79 O/C(=N\nnc(-c2ccccc2)o1)c1ccccc1

80 OP(=Nc1nnc(-c2ccccc2)o1)(c1ccccc1)c1ccccc1

81 Oc1ccccc1-c1nc2ccccc2o1

82 Oc1ccccc1-c1ncco1

83 Oc1ccccc1-c1nccs1

84 O=C(O)c1ccccn1

85 c1ccc(Cn2c(-c3ccccc3)nc3ccccc32)cc1

86 Fc1ccc(Cn2c(-c3ccc(F)cc3)nc3ccccc32)cc1

87 Cc1ccc(Cn2c(-c3ccc(C)cc3)nc3ccccc32)cc1

88 COc1ccc(Cn2c(-c3ccc(OC)cc3)nc3ccccc32)cc1

89 Cn1c(=O)c2c(F)cccc2c2ncccc21

90 Cn1c(=O)c2cc(C(F)(F)F)ccc2c2ncccc21

91 O=C(O)c1cnccn1

92 FC(F)(F)c1ccc(-c2nc3c4ccccc4c4ccccc4c3n2-c2ccccc2)cc1

93 Cc1ccc(-n2c(-c3ccc(C(F)(F)F)cc3)nc3c4ccccc4c4ccccc4c32)cc1

94 COc1ccc(-n2c(-c3ccc(C(F)(F)F)cc3)nc3c4ccccc4c4ccccc4c32)cc1

95 Cc1cc(C)cc(-n2c(-c3ccc(C(F)(F)F)cc3)nc3c4ccccc4c4ccccc4c32)c1

96 CN(C)c1ccnc(C(=O)O)c1

97 Cc1cc(C)c(-c2ccccn2)[nH]1

98 c1ccc(-c2cc(-c3ccccc3)c(-c3ccccn3)[nH]2)cc1

99 FC(F)(F)c1cc(C(F)(F)F)c(-c2ccccn2)[nH]1

100 Cc1ccc(N2C=CN(C)C2)cc1

101 c1ccc(-c2nc3ccccc3[nH]2)nc1

102 c1ccc(-c2nc3ccccc3n2-c2ccccc2)cc1

103 Cc1n[nH]c(-c2ccccn2)n1

104 c1ccc(-c2ncc[nH]2)nc1

105 c1ccc(-c2ccn[nH]2)nc1

106 Cc1ccnc(-c2ccn[nH]2)c1

107 c1ccc(-c2nnn[nH]2)nc1

108 Cc1ccc(-c2nc3ccccc3n2-c2ccccc2)cc1

109 CC(C)(C)c1ccc(-c2nc3ccccc3n2-c2ccccc2)cc1

110 Cc1cc(-c2ccccn2)[nH]n1

111 c1ccc(-c2cc(-c3ccccn3)[nH]n2)cc1

112 FC(F)(F)c1cc(-c2ccccn2)[nH]n1

113 c1ccc(-c2cc(-c3ccncc3)n[nH]2)nc1

114 c1ccc(-c2cc(-c3ccccc3)ncn2)cc1

115 FC(F)(F)c1n[nH]c(-c2ccccn2)n1

116 Cc1cc(C)cc(-c2n[nH]c(-c3ccccn3)n2)c1

117 c1ccc(-c2n[nH]c(-c3ccccn3)n2)cc1

118 Fc1ccc(-c2n[nH]c(-c3ccccn3)n2)cc1

119 Fc1cc(F)cc(-c2n[nH]c(-c3ccccn3)n2)c1

120 Fc1c(F)c(F)c(-c2n[nH]c(-c3ccccn3)n2)c(F)c1F

121 C1=CC2c3ccccc3N(CCCCCCCCc3ccccc3-c3nc4ccccc4s3)C2C=C1

122 Cc1cc(-c2ccccc2)nc2ccccc12

123 Cc1cc(-c2ccc(F)cc2)nc2ccccc12

124 Cc1cc(-c2ccc(F)cc2F)nc2ccccc12

125 Cc1cc(-c2ccc(F)c(F)c2F)nc2ccccc12

126 Cc1cc(-c2cc(F)cc(F)c2)nc2ccccc12

127 Cc1cc(-c2cc(F)c(F)c(F)c2)nc2ccccc12

128 Cc1cc(-c2cc(F)c(F)c(F)c2F)nc2ccccc12

129 Cc1cc(-c2cccc(C(F)(F)F)c2)nc2ccccc12

130 Cc1cc(-c2ccc(F)c(C(F)(F)F)c2)nc2ccccc12

131 FC(F)(F)c1nnc(-c2ccccn2)[nH]1

132 c1ccc(/N=c2/cccc[nH]2)nc1

133 CC(C)[N]/C(=N/C(C)C)c1ccccc1

134 CC(C)(C)[N]/C(=N/C(C)(C)C)c1ccccc1

135 CC/N=C(/[N]C(C)(C)C)c1ccccc1

136 CC/N=C(/[N]CCCN(C)C)c1ccccc1

137 CC(C)[N]/C(=N/C(C)C)n1c2ccccc2c2ccccc21

138 CC(C)[N]/C(=N/C(C)C)n1c2ccc(C(C)(C)C)cc2c2cc(C(C)(C)C)ccc21

139 CC(C)[N]/C(=N/C(C)C)N1c2ccccc2Sc2ccccc21

140 CC(C)[N]/C(=N/C(C)C)N1c2ccccc2Oc2ccccc21

141 CC(C)[N]/C(=N/C(C)C)n1ccc2ccccc21

142 CCN(CC)/C([N]C(C)C)=N(C)C

143 CC(C)[N]/C(=N/C(C)C)N(C(C)C)C(C)C

144 CC(C)CN(CC(C)C)/C([N]C(C)C)=N(C)C

145 CC(C)[N]/C(=N/C(C)C)N([Si](C)(C)C)[Si](C)(C)C

146 FC(F)(F)c1cc(-c2cc(C(F)(F)F)n[nH]2)[nH]n1

147 CC(C)(C)c1ccnc(-c2cc(C(C)(C)C)ccn2)c1

148 CC(C)(C)c1cc(C(C)(C)c2cc(C(C)(C)C)n[nH]2)[nH]n1

149 CN1[CH]N(c2ccccc2)C=C1

150 CN1[CH]N(c2ccccc2)c2ccccc21

151 CN1[CH]N(c2ccccc2)c2ncccc21

152 CCN1[CH]N(c2ccc(C(C)(C)C)cc2)c2ncccc21

153 CN1[CH]N(c2cccc3c2oc2ccccc23)C=C1

154 CC(C)c1cc2c(oc3ccccc32)c(C(C)C)c1N1C=CNC1c1ccccc1

155 CCCCN1C=CNC1c1ccc(F)cc1

156 CCCCN1C=CNC1c1ccc(OC(F)(F)F)cc1

157 CCCCN1C=CNC1c1ccc(C(F)(F)F)cc1

158 Cc1cc(C)c(N2C=CNC2c2ccccc2)c(C)c1

159 Cc1cccc(C)c1N1C=CNC1c1ccccc1

160 CC(C)c1cccc(C(C)C)c1N1C=CNC1c1ccccc1

161 CC(C)c1cc(-c2ccccc2)cc(C(C)C)c1N1C=CNC1c1ccccc1

162 Fc1ccc(C2NC=CN2c2c(-c3ccccc3)cccc2-c2ccccc2)cc1

163 Cc1cc(-c2ccccc2)c(N2C=CNC2c2ccc(F)cc2)c(-c2ccccc2)c1

164 CCCc1cc(-c2ccccc2)c(N2C=CNC2c2ccc(F)cc2)c(-c2ccccc2)c1

165 CC1=NN(C)C(c2ccccc2)N1

166 Fc1ccc(-c2ccccn2)c(F)n1

167 COc1ccc(-c2cc(C)ccn2)c(OC)n1

168 COc1ccnc(-c2ccc(OC)nc2OC)c1

169 CN1C=CN(c2ccc(F)cc2)C1

170 Cc1cnc(-c2ccn[nH]2)c(C)c1

171 Fc1ccc(-c2ccccn2)c(F)c1

172 CN1C=CN(c2ccc(C(F)(F)F)cc2)C1

173 CN1CN(c2ccc(C(F)(F)F)cc2)c2ccccc21

174 CN1C=CN(c2cccc(C(F)(F)F)c2)C1

175 COc1ccc(N2C=CN(C)C2)c(OC)c1

176 COc1ccc(N2C=CN(C)C2)c(OC)n1

177 COc1ccc(N2C=CN(C)C2)c(C)n1

178 COc1ccc(N2CN(C)C=N2)c(OC)c1

179 O=P(c1ccccc1)(c1ccccc1)c1c(F)ccc(-c2ccccn2)c1F

180 O=S(=O)(c1ccccc1)c1c(F)ccc(-c2ccccn2)c1F

181 O=C(c1ccccc1)c1c(F)ccc(-c2ccccn2)c1F

182 Cc1ccnc(-c2ccc(F)c(C(=O)C(F)(F)F)c2F)c1

183 Cc1ccnc(-c2ccc(F)c(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c2F)c1

184 Cc1ccnc(-c2ccc(F)c(C(F)(F)C(F)(F)C(F)(F)F)c2F)c1

185 Cc1ccnc(C(=O)O)c1

186 CCOc1ccc(-c2cc(C)ccn2)c(F)c1F

187 Cc1ccnc(-c2ccc(F)cc2F)c1

188 O=C(O)C1=CC=CCN1O

189 Cc1ccnc(-c2ccc(F)c(C(F)(F)F)c2F)c1

190 CC(C)(C)c1ccnc(-c2ccc(F)c(CN)c2F)c1

191 Oc1ccccc1C1=NCCO1

192 C[Si](C)(C)c1ccc(-c2ccc(F)cc2F)nc1

193 FC(F)(F)C(F)(F)C(F)(F)c1n[nH]c(-c2ccccn2)n1

194 C[Si](C)(C)c1ccnc(-c2ccc(F)cc2F)c1

195 O=P(O)(c1ccccc1)c1ccccn1

196 O=P(O)(c1ccccn1)c1ccccn1

197 CC(C)(C)c1ccnc(-c2ccc(F)nc2F)c1

198 CC(C)(C)c1ccnc(-c2cc(C(F)(F)F)n[nH]2)c1

199 Cc1ccnc(-c2ccc(F)nc2F)c1

200 COc1ccnc(-c2ccc(F)nc2F)c1

201 O=P(CP(=O)(c1ccccc1)c1ccccc1)(c1ccccc1)c1ccccc1

202 O=P(CP(=O)(c1ccc(F)cc1)c1ccc(F)cc1)(c1ccc(F)cc1)c1ccc(F)cc1

203 COc1ccc(-c2cc(C(C)(C)C)ccn2)c(OC)n1

204 COc1ncc(-c2cc(C(C)(C)C)ccn2)c(OC)n1

205 CC(C)(C)c1ccnc(-c2[nH]c(C(F)(F)F)cc2C(F)(F)F)c1

206 FC(F)(F)c1ncc(-c2ccccn2)cn1

207 c1ccc(-n2cccn2)cc1

208 FC(F)(F)c1ccc(-c2n[nH]c(-c3ccccn3)n2)cc1

209 Fc1ccc(-c2cn(Cc3ccccc3)nn2)c(F)c1

210 Cc1ccc(-c2nc(C)nn2C)cc1

211 Cc1ccnc(-c2ncn[nH]2)c1

212 CCCc1nc(-c2ccc(C)cc2)n(C)n1

213 c1ccc(-c2ncn[nH]2)nc1

214 CC(C)(C)c1n[nH]c(-c2ccccn2)n1

215 c1ccc(CP(c2ccccc2)c2ccccc2)cc1

216 c1ccc(OP(c2ccccc2)c2ccccc2)cc1

217 c1ccc(-c2cc(-c3cccs3)nc3ccccc23)cc1

218 c1ccc(-c2cc(-c3ccc[se]3)nc3ccccc23)cc1

219 FC(F)(F)c1ccc(-c2nnc(-c3cccs3)c3cc4ccccc4cc23)c(C(F)(F)F)c1

220 c1csc(-c2nnc(-c3cccs3)c3cc4ccccc4cc23)c1

221 CCCC(CC)COc1ccc(-n2c3ccccc3c3cc(-c4cc(-c5ccccc5)c5ccccc5n4)ccc32)cc1

222 c1ccc(N(c2ccccc2)c2cccc(-c3ccnc(-c4cccc(N(c5ccccc5)c5ccccc5)c4)c3)c2)cc1

223 CCCc1ccc2c(c1)c1cc(CCC)ccc1n2-c1ccc(-c2ccc(-c3cc(-c4cccs4)nc4ccccc34)cc2)cc1

224 CCC1(CC)c2ccccc2-c2cc(-c3ccc(C(F)(F)F)cn3)ccc21

225 CCC1(CC)c2ccccc2-c2cc(-c3nccs3)ccc21

226 c1ccc2c(-c3nccs3)cccc2c1

227 c1ccc2cc(-c3nccs3)ccc2c1

228 c1ccc(-n2c3ccccc3c3cc(-c4ccccn4)ccc32)cc1

229 c1ccc(-n2c3ccccc3c3ccc(-c4ccccn4)cc32)cc1

230 c1ccc(-n2c3ccccc3c3cc(-c4nccs4)ccc32)cc1

231 CC(C)N1C(=O)c2ccc(-c3ccccn3)cc2C1=O

232 c1ccc(-c2ccc3c(-c4ccccc4)cccc3n2)cc1

233 Fc1cccc2nc(-c3ccccc3)ccc12

234 Fc1ccc(-c2cccc3nc(-c4ccccc4)ccc23)cc1

235 CC1(C)c2cc(-c3ccc4c(-c5ccccc5)cccc4n3)ccc2C2C=CC=CC21

236 CC1(C)c2cc(-c3ccc4c(F)cccc4n3)ccc2C2C=CC=CC21

237 CC1(C)c2cc(-c3ccc4c(-c5ccc(F)cc5)cccc4n3)ccc2C2C=CC=CC21

238 c1ccc(-c2ccc3nc(-c4ccccc4)ccc3c2)cc1

239 Fc1ccc(-c2ccc3nc(-c4ccccc4)ccc3c2)cc1

240 c1ccc(-c2ccc3nc(-c4ccccc4)cc(-c4ccccc4)c3c2)cc1

241 c1ccc(-c2ccc3ccccc3n2)cc1

242 c1ccc(-c2ccc(-c3ccccn3)cc2)cc1

243 Cc1cc(C)cc(-c2ccc3ccccc3n2)c1

244 CCC1(C)c2cc(-c3ccc(C(F)(F)F)cn3)ccc2C2C=CC=CC21

245 O=C(CC(=O)c1ccccc1)c1ccccc1

246 CCC1(CC)c2cc(-c3ccc(C(F)(F)F)cn3)ccc2C2C=CC=CC21

247 c1ccc2sc(-c3nccc4ccccc34)cc2c1

248 O=C(CC(=O)C(F)(F)F)c1cccs1

249 O=C(CC(=O)c1cccs1)c1cccs1

250 Cc1nc2cc3ccccc3cc2nc1-c1ccccc1

251 O=S1(=O)c2ccccc2-c2cc(-c3nc4ccccc4s3)ccc21

252 O=P(c1ccccc1)(c1ccccc1)c1ccc(-c2nc3ccccc3s2)cc1

253 c1ccc(-n2c3ccccc3c3ccc(-c4nc5ccccc5s4)cc32)cc1

254 CCn1c2ccccc2c2cc3nc(-c4ccccc4)sc3cc21

255 c1ccc(-c2nc3cc4c(cc3s2)oc2ccccc24)cc1

256 c1ccc(-c2nc3cc4ccccc4cc3s2)cc1

257 c1csc(-c2ncc3ccccc3n2)c1

258 c1ccc(N(c2ccccc2)c2nc(-c3cccs3)nc3ccccc23)cc1

259 CCc1cc(C)cc(-c2cc(-c3cc(C)cc(C)c3)ncn2)c1

260 CC(C)(C)c1ccc(-c2nc3ccccc3c3ccccc23)cc1

261 CC(C)(C)c1ccc(N(c2ccc(-c3nc4ccccc4c4ccccc34)cc2)c2ccc(C(C)(C)C)cc2)cc1

262 FC(F)(F)c1cc(-c2nccc3ccccc23)cc(C(F)(F)F)n1

263 FC(F)(F)c1cc(-c2ncnc3ccccc23)cc(C(F)(F)F)n1

264 c1ccc(-c2nc3ccccc3nc2-c2ccccc2)cc1

265 Fc1cc2nc(-c3ccccc3)c(-c3ccccc3)nc2cc1F

266 Fc1ccc(-c2nc3ccccc3nc2-c2ccc(F)cc2)cc1

267 Fc1ccc(-c2nc3cc(F)c(F)cc3nc2-c2ccc(F)cc2)cc1

268 CCCCCCc1csc(-c2ccc(-c3cc(CCCCCC)cs3)nc2)c1

269 CCC1(CC)c2cc(-c3ccc(C(F)(F)F)cn3)ccc2-c2ccc(N(c3ccc(OC)cc3)c3ccc(OC)cc3)cc21

270 Cc1cc(-c2cccs2)nc2ccccc12

271 c1ccc(N(c2ccccc2)c2ccc(-c3nc4ccccc4s3)cc2)cc1

272 c1c[nH]c(-c2nccc3ccccc23)c1

273 c1ccc2c(c1)ccc1cccnc12

274 Fc1ccc(-c2nccc3ccccc23)cc1

275 Fc1ccc(-c2nccc3ccccc23)c(F)c1

276 CCN(CC)C(=S)S

277 Cc1cc(C)c(C(c2ccc(-c3ccccn3)cc2)c2c(C)cc(C)cc2C)c(C)c1

3D information of candidates with red, yellow, green and blue colors

The 3D information of candidates with red, yellow, green and blue colors can be obtained from https://github.com/zhengcheng233/Ir_complexs

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