

Table S1. Formal names of iridium complexes

Complex	Formal name
<i>fac</i> -Ir(ppy) ₃	<i>fac</i> -tris(2-phenylpyridinato-N,C ^{2'})iridium(III)
<i>mer</i> -Ir(ppy) ₃	<i>mer</i> -tris(2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dF-ppy) ₃	<i>fac</i> -tris(4',6'-difluoro-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(5'-CN-4',6'-dF-ppy) ₃	<i>fac</i> -tris(5'-cyano-4',6'-difluoro-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(1,3-pdz) ₃	<i>fac</i> -tris(2-phenyl-1,3-diazinato-N,C ^{2'})iridium(III)
Ir(1,4-pdz) ₃	<i>fac</i> -tris(2-phenyl-1,4-diazinato-N,C ^{2'})iridium(III)
Ir(1,5-pdz) ₃	<i>fac</i> -tris(4-phenyl-1,3-diazinato-N,C ^{2'})iridium(III)
Ir(1,6-pdz) ₃	<i>fac</i> -tris(3-phenyl-1,2-diazinato-N,C ^{2'})iridium(III)
Ir(2,3'-bpy) ₃	<i>fac</i> -tris(2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(2,4'-bpy) ₃	<i>fac</i> -tris(2,4'-bipyridinato-N,C ^{2'})iridium(III)
Ir(2,5'-bpy) ₃	<i>fac</i> -tris(2,5'-bipyridinato-N,C ^{2'})iridium(III)
Ir(2,6'-bpy) ₃	<i>fac</i> -tris(2,6'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dF-2,5'-bpy) ₃	<i>fac</i> -tris(4,6-difluoro-2,5'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dNH ₂ -2,5'-bpy) ₃	<i>fac</i> -tris(4,6-diamino-2,5'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dOH-2,5'-bpy) ₃	<i>fac</i> -tris(4,6-dihydroxy-2,5'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dF-2,3'-bpy) ₃	<i>fac</i> -tris(4,6-difluoro-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dNH ₂ -2,3'-bpy) ₃	<i>fac</i> -tris(4,6-diamino-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dOH-2,3'-bpy) ₃	<i>fac</i> -tris(4,6-dihydroxy-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(5'-CN-2,3'-bpy) ₃	<i>fac</i> -tris(5-cyano-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(5'-NO ₂ -2,3'-bpy) ₃	<i>fac</i> -tris(5-nitro-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dF-5'-CN-2,3'-bpy) ₃	<i>fac</i> -tris(4,6-difluoro-5-cyano-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dF-5'-NO ₂ -2,3'-bpy) ₃	<i>fac</i> -tris(4,6-difluoro-5-nitro-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dNH ₂ -5'-CN-2,3'-bpy) ₃	<i>fac</i> -tris(4,6-diamino-5-cyano-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4',6'-dOH-5'-CN-2,3'-bpy) ₃	<i>fac</i> -tris(4,6-dihydroxy-5-cyano-2,3'-bipyridinato-N,C ^{2'})iridium(III)
Ir(4'-NH ₂ -ppy) ₃	<i>fac</i> -tris(4'-amino-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(6'-NH ₂ -ppy) ₃	<i>fac</i> -tris(6'-amino-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(4'-OH-ppy) ₃	<i>fac</i> -tris(4'-hydroxy-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(6'-OH-ppy) ₃	<i>fac</i> -tris(6'-hydroxy-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(4'-NMe ₂ -ppy) ₃	<i>fac</i> -tris(4'-dimethylamino-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(6'-NMe ₂ -ppy) ₃	<i>fac</i> -tris(6'-dimethylamino-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(4'-OMe-ppy) ₃	<i>fac</i> -tris(4'-methoxy-2-phenylpyridinato-N,C ^{2'})iridium(III)
Ir(6'-OMe-ppy) ₃	<i>fac</i> -tris(6'-methoxy-2-phenylpyridinato-N,C ^{2'})iridium(III)