

## Cross coupling Genome

They present sketch-maps for **25,112 catalysts**, categorized by metal type. Each catalyst's name is expressed in the form metal\_L1\_L2 and is colored by the value of its energy-based descriptor (i.e., substrate binding energy) for different cross-coupling reactions. The color code corresponds to the volcano plateau of the different reactions, where black represents the plateau region for Suzuki coupling. Green and red shades (see color bar) indicate catalysts with ideal thermodynamics (i.e., species that fall of the plateau) for other cross-coupling reactions (i.e., Kumada, Negishi, Stille, and Hiyama). Catalysts depicted in gray are not ideal for any of the coupling reactions studied.

The chemical structures of the 91 ligands are available in the [archive record](#).