The following plots correspond to Figure 5 in the section “**Capturing Chemical Reaction Diversity**” (which is based on Reaxys data) specifically analysing the USPTO dataset.

A graph of a bar chart

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**Figure 5a: Suzuki Coupling Reactions—USPTO**

The distribution observed here closely mirrors the trends in the Reaxys dataset described in the main manuscript. Notably, the USPTO data reveals a pronounced increase in the diversity of the halide chemical environments involved in Suzuki coupling reactions. However, the onset of this increase is temporally distinct: while the Reaxys dataset indicates a sharp rise in diversity between 1994 and 1997, the USPTO dataset suggests this shift occurred later, around 2000 to 2003.

**Figure 5b: C–C Decarboxylative Coupling Reactions—USPTO**

In contrast to the Suzuki plot and corresponding Reaxys data, the number of USPTO entries for C–C decarboxylative coupling reactions is markedly lower—only **94 usable data points** were identified in this dataset. Due to the limited sample size, no meaningful trends are discussed for this reaction type.

A graph of a bar chart

AI-generated content may be incorrect.

Figure 5. Distribution of the USPTO reaction data with res pect to the years (binned per 2 years for enhancing the plot clarity, for 2 reaction types (a) Suzuki, (b) C–C decarboxylative coupling. The numbers in the bars indicate the number of unique SMARTS-RX, the colour classification is related to the ontology level 2.