Supplementary Information

One Step Retrosynthesis of Drugs from Commercially Available Chemical Building Blocks and Conceivable Coupling Reactions

Figure S1 – Figure 2 Venn analysis excluding C-H coupling building block pairs

Figure S2 – Figure 4 chord plots excluding C-H coupling building block pairs

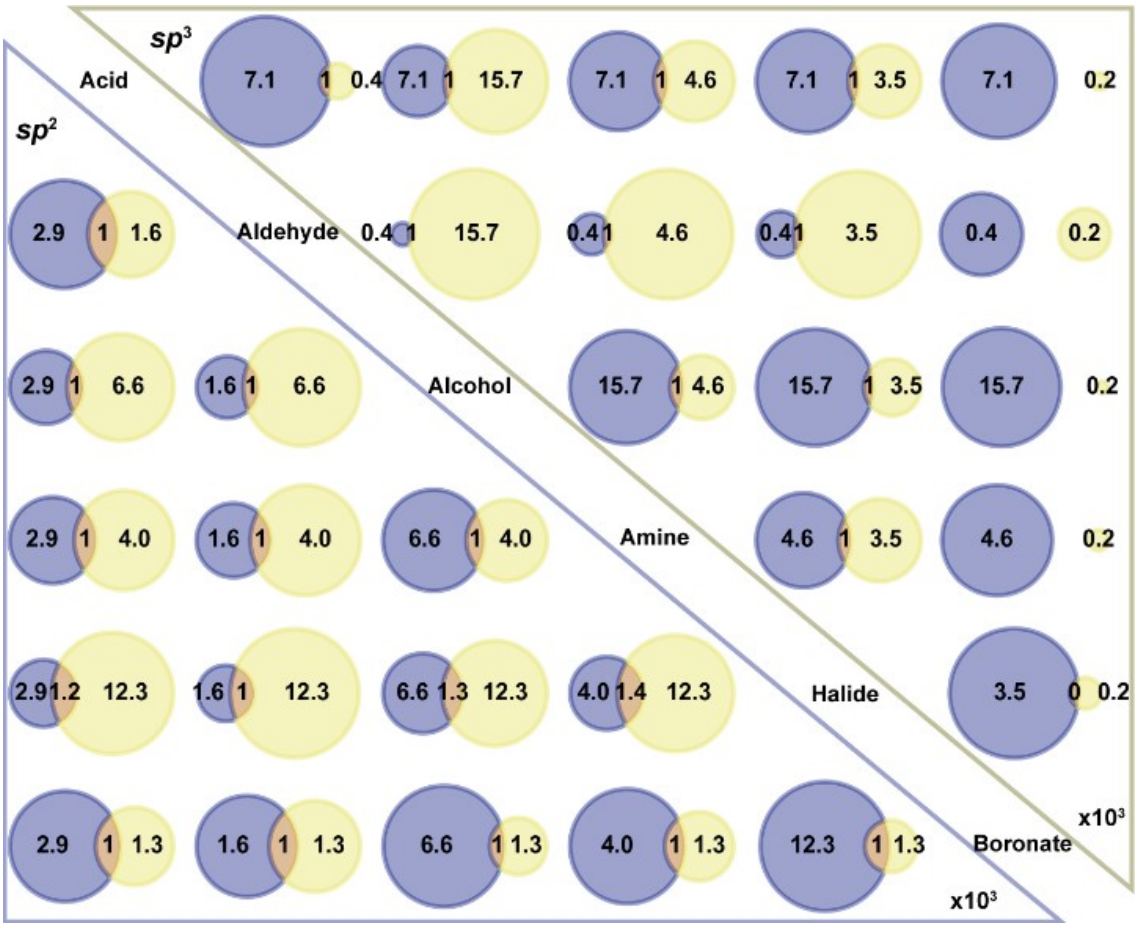

Figure S1. Bottom left: Venn analysis excluding C-H couplings of shared and disparate core structures of commercially available sp^2 compounds. The values in the purple (left) circles indicate the number of core structures in the building block class above that do not exist in the building block class on the right, and vice versa for the values in the yellow (right) circles. The orange overlapping section indicates the number of shared structures between the two classes. Top right: Venn analysis of shared (purple, left label – yellow, bottom label) vs disparate core structures (overlapping, orange) of commercially available sp^3 compounds. Each occurrence of a functional group in a building block is counted.

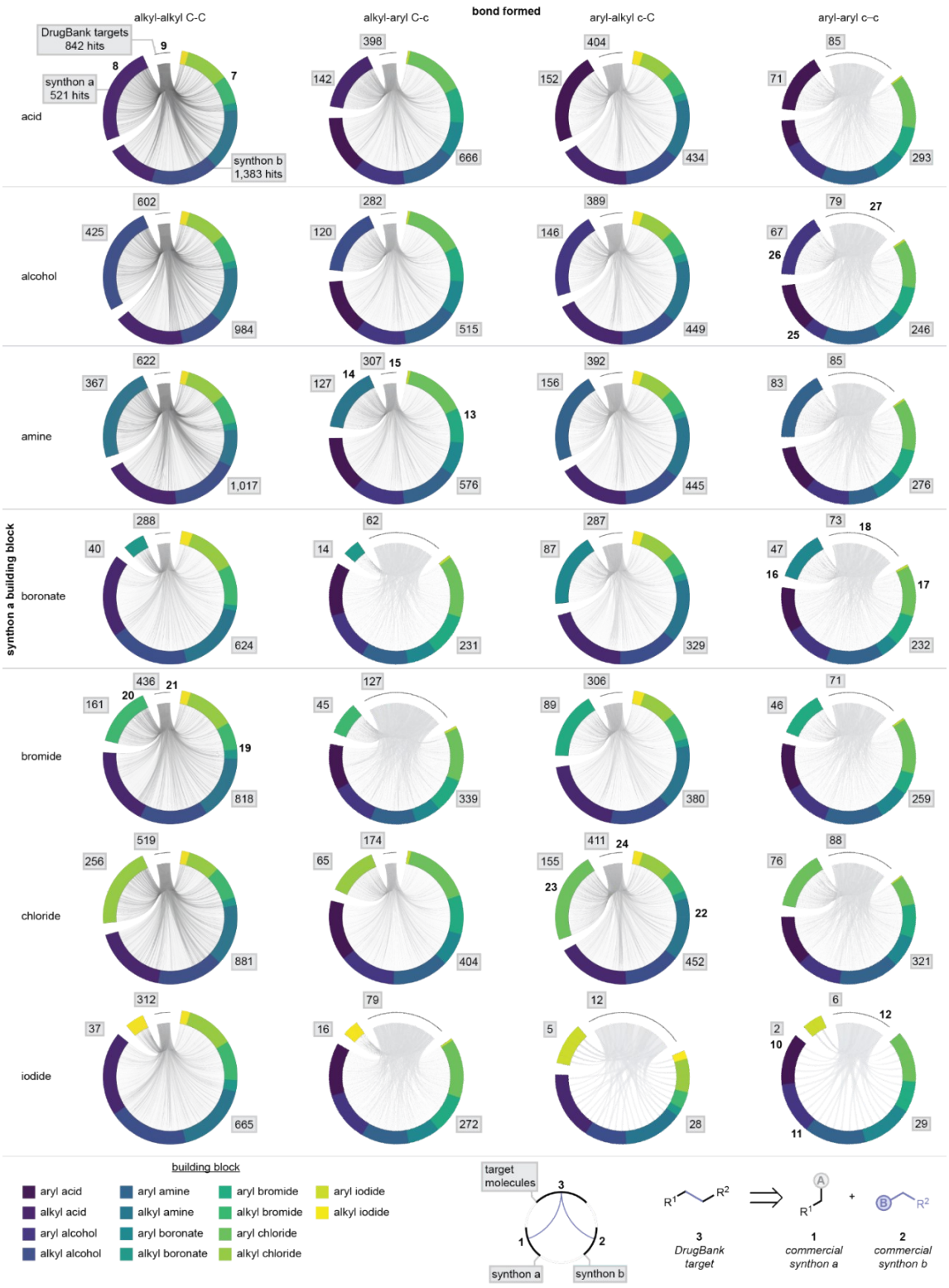

Figure S2. Single-step C-H excluded cross-coupling maps between DrugBank and purchasable compounds in Sigma-Aldrich's catalog trellised by synthon A building block and bond formed. In the first column, both synthons link at an alkyl carbon. In the second column, synthon A, which is the building block group for the row, is alkyl and the remaining synthon b is aryl. In the third column, the building block arc contains aryl synthons and synthon b contains alkyl synthons. In the final column, both synthons are aryl. Compound numbers refer to retrosynthetic reactions shown in Figure 3.