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Molecular Shape Diversity of Combinatorial Libraries: a Prerequisite for Broad Bioactivity

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Individual shape triangle diagrams obtained by plotting the envelope shapes of the respective compounds belonging to libraries S_1 – S_{50} (Chart 1), S_{51} – S_{65} (Chart 2), and the MDDR biological activity subsets (Chart 3), using the methods outlined in the Methodology section. For details on the nomenclature, as well as the scaffold and building block choice, used for libraries S_1 – S_{65} , the reader is referred to Table 1, and Figures 3–5 in the main text. The corresponding numerical pairwise similarity values associated with the triangle graphs of the compound sets shown in Chart 1, Chart 2, and Chart 3 are to be found in the main text, in Tables 2, 4, and 5, respectively.

Chart 1. Shape triangle diagrams of the 50 sub-libraries of library (C), **S**₁–**S**₅₀, derived according to Table 1 from scaffolds **A**₁–**A**₅₀ (see Figure 4) and substituents **B**₅, **B**₆, **B**₁₁, **B**₁₈, **B**₂₇, **B**₂₉, **B**₃₂, **B**₄₁, **B**₄₃, **B**₄₅, **B**₄₇, **B**₄₈, **B**₅₀ (see Figure 3).

Chart 1. (continued)

Chart 1. (continued)

Chart 2. Shape triangle diagrams of two-point diversity minimal libraries, **S**₅₁–**S**₆₅, derived according to Table 1 from scaffolds **A**₅₁–**A**₆₅ (see Figure 5) and substituents **B**₁–**B**₅₀ (see Figure 3).

Chart 3. Shape triangle diagrams of MDDR subsets grouped by biological activities (see Table 5).

Chart 3. (continued)