A Library of Tunable Saturated *N*-Heterocycles Enabled by Reaction Outcome and Property Predictions

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We present a library of morpholines and piperazines obtained from the silicon amine protocol (SLAP) reaction. This reaction utilizes widely available aldehyde and ketone building blocks to give *N*-heterocycles with diverse substituents. We use a 96-well photoreactor, combined with high-throughput prep-HPLC and analysis by LCMS, CAD, and qNMR to evaluate 900 reactions. Alongside, aqueous solubility, log *D*, and pK_a measurements are obtained for the isolated compounds. We construct a virtual library based on commercially available building blocks and train graph neural networks (GNN) to predict synthesizability and physicochemical properties of the products based on our data. The GNN-annotated virtual library enables rational selection and high-throughput exploration of subsets from a pool of 20 million diverse *N*-heterocycles.