

Supplementary Information

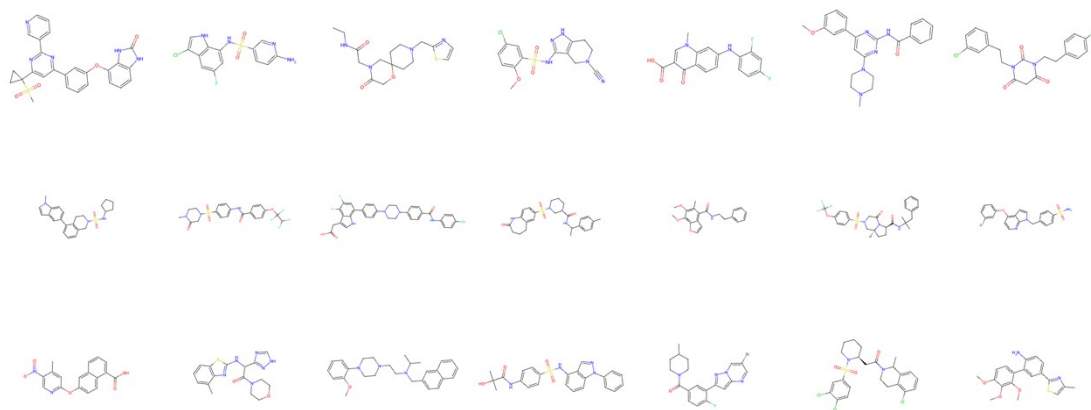


Fig. S1. Visualization of molecules generated in the de novo design task.

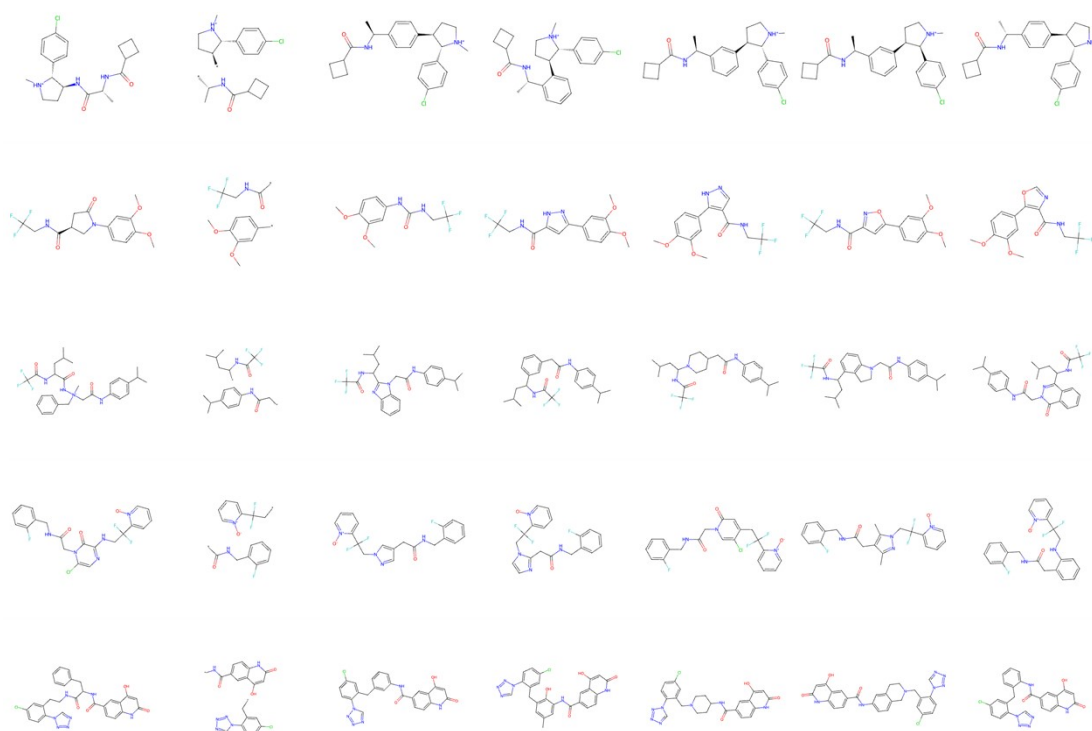


Fig. S2. Visualization of molecules generated in the linker design task. The first column illustrates the reference molecules, the second column depicts the retained segments, and the subsequent columns showcase the newly generated molecules.

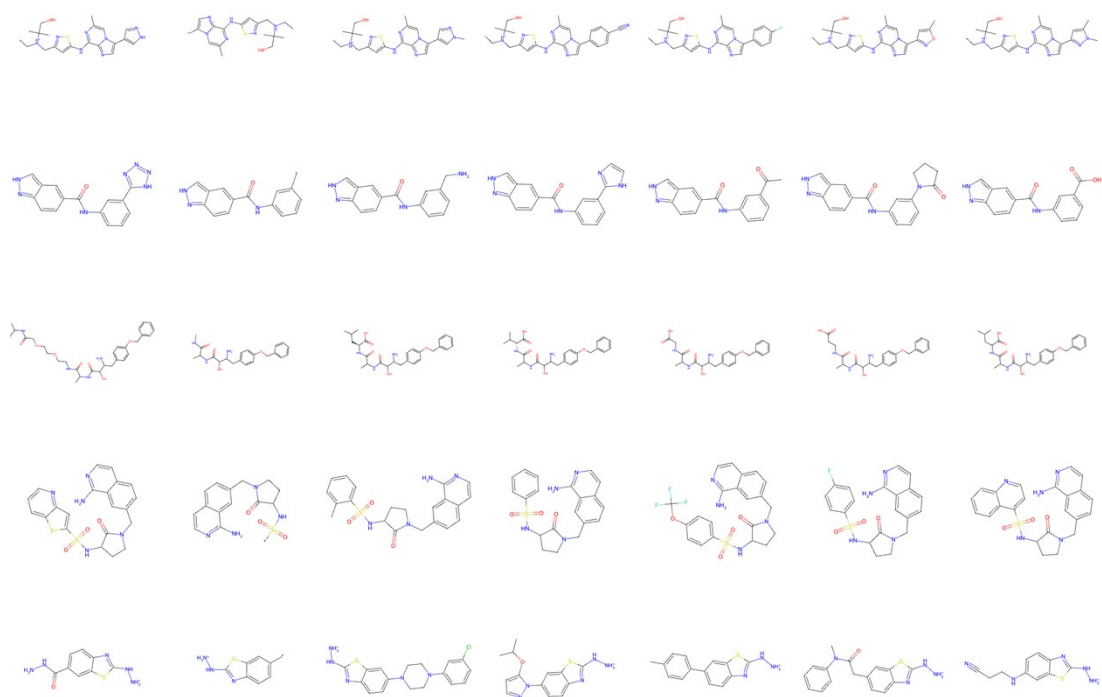


Fig. S3. Visualization of molecules generated in the R-group exploration task. The first column illustrates the reference molecules, the second column depicts the retained segments, and the subsequent columns showcase the newly generated molecules.

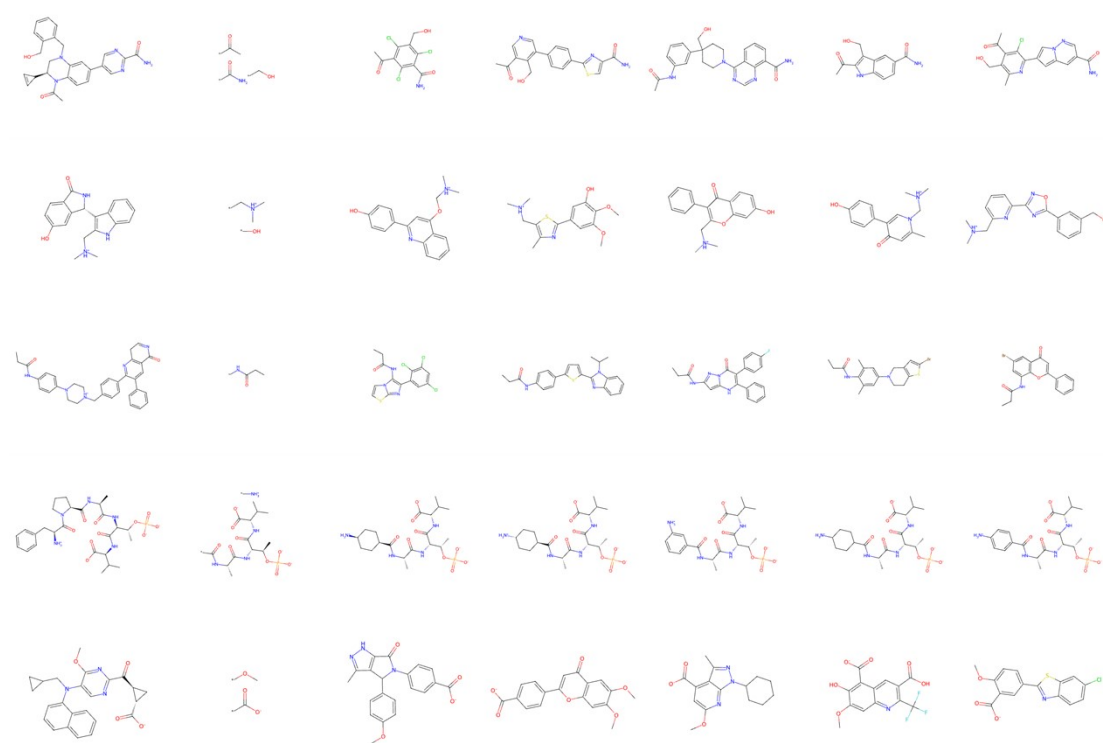


Fig. S4. Visualization of molecules generated in the scaffold hopping task. The first column illustrates the reference molecules, the second column depicts the retained segments, and the subsequent columns showcase the newly generated molecules.

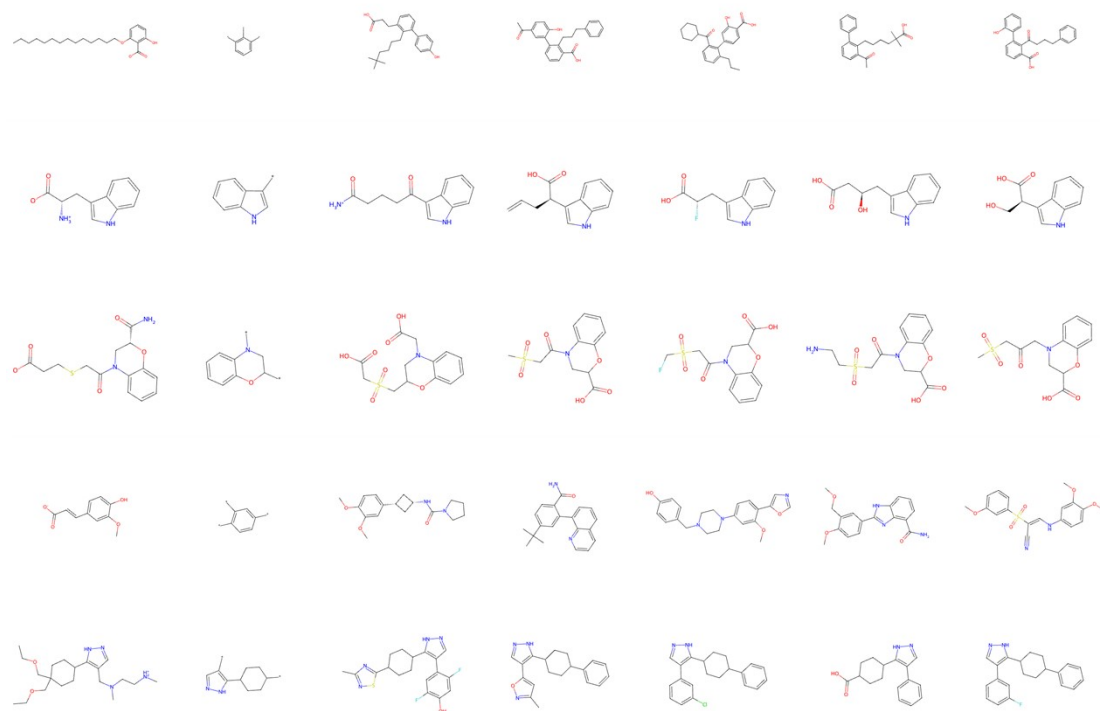


Fig. S5. Visualization of molecules generated in the side chain optimization task. The first column illustrates the reference molecules, the second column depicts the retained segments, and the subsequent columns showcase the newly generated molecules.