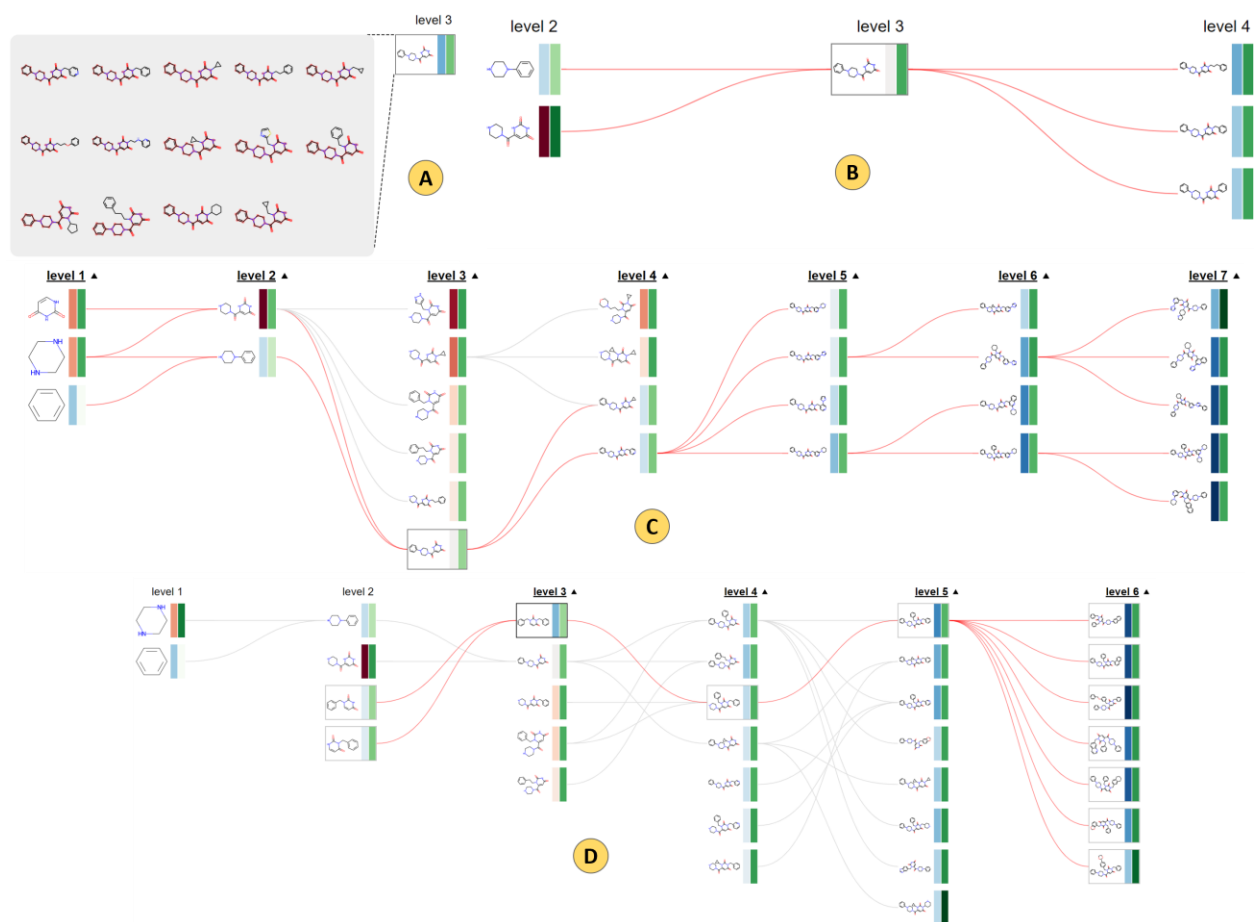


This document shows the results from various key steps involved in the usage scenario explained in the paper.



Process of generating SAR series from a lead compound with key steps: (A): Load the lead molecule to start exploration from the scaffold class of the lead molecule. (B): Running *upper* and *lower* operations once with a sample size of 3, to expand the scaffold network on both sides. (C), (D): Two different scaffold graphs are generated by choosing different scaffolds based on specific properties of preference at each step. Each scaffold graph results in a different SAR series. The one in (c) is generated by choosing compounds that are easy to dissolve whereas the one in (d) is results in compounds that are easily synthesizable.