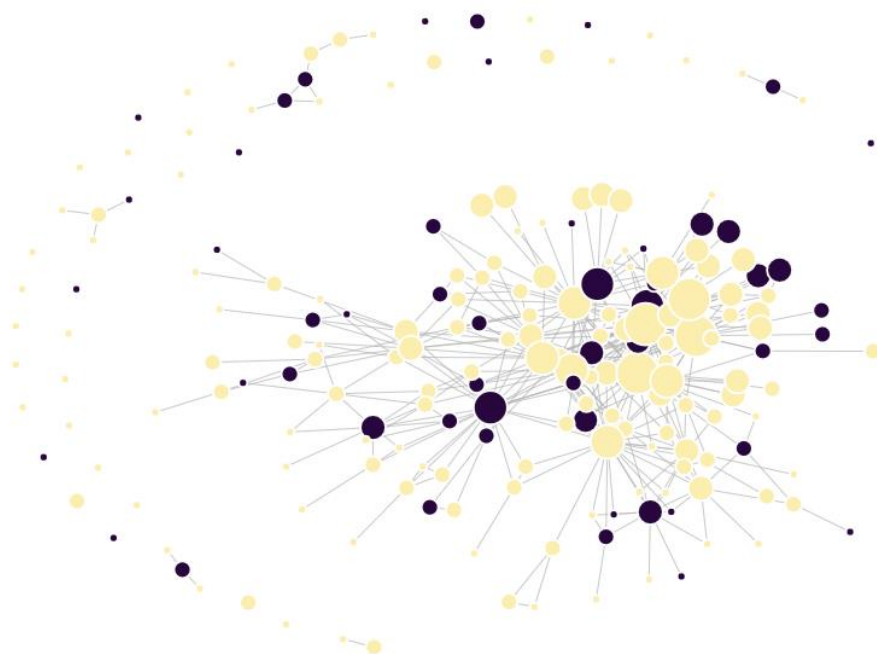
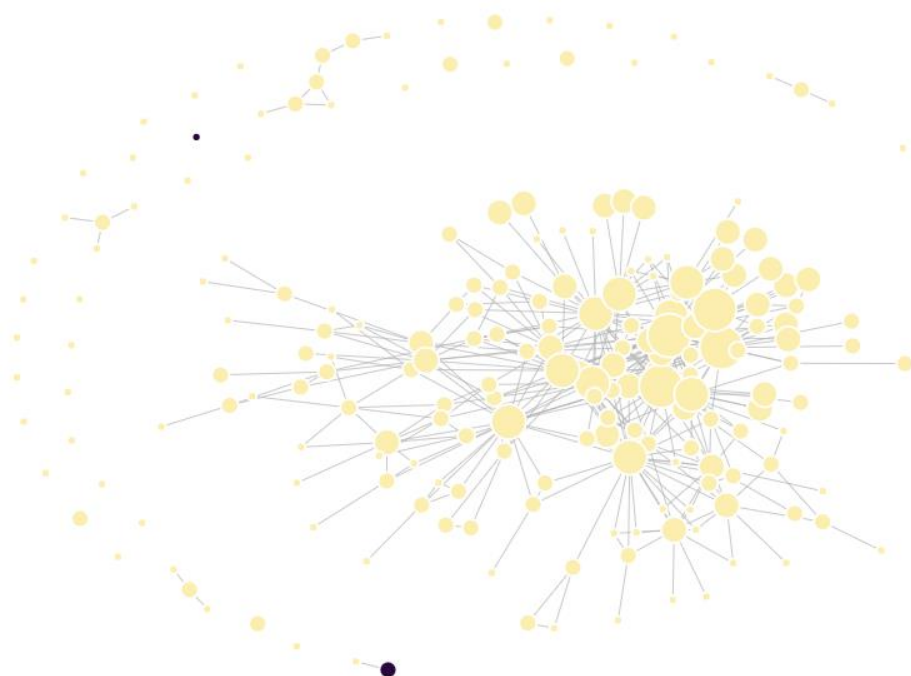


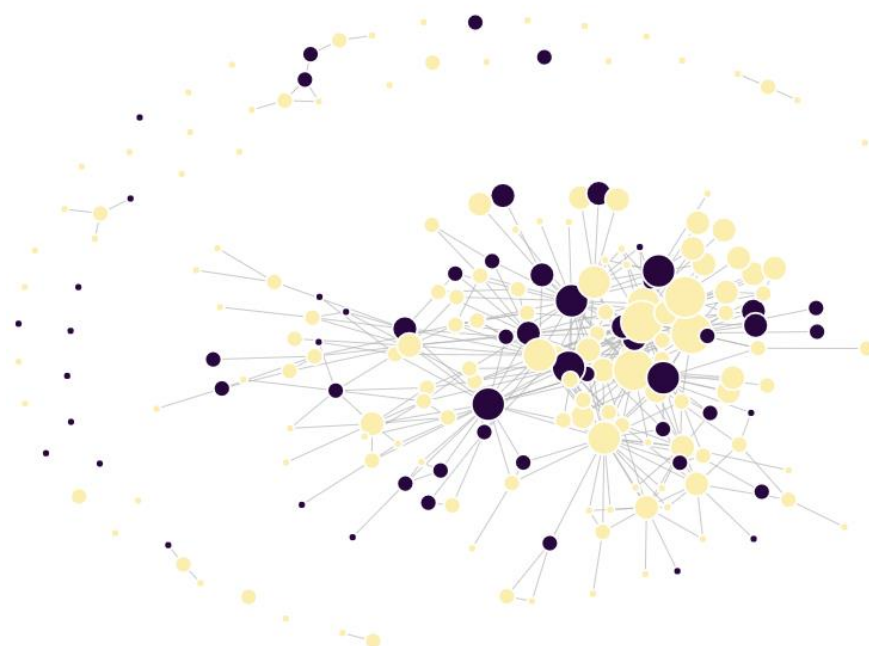
A



B



C



D

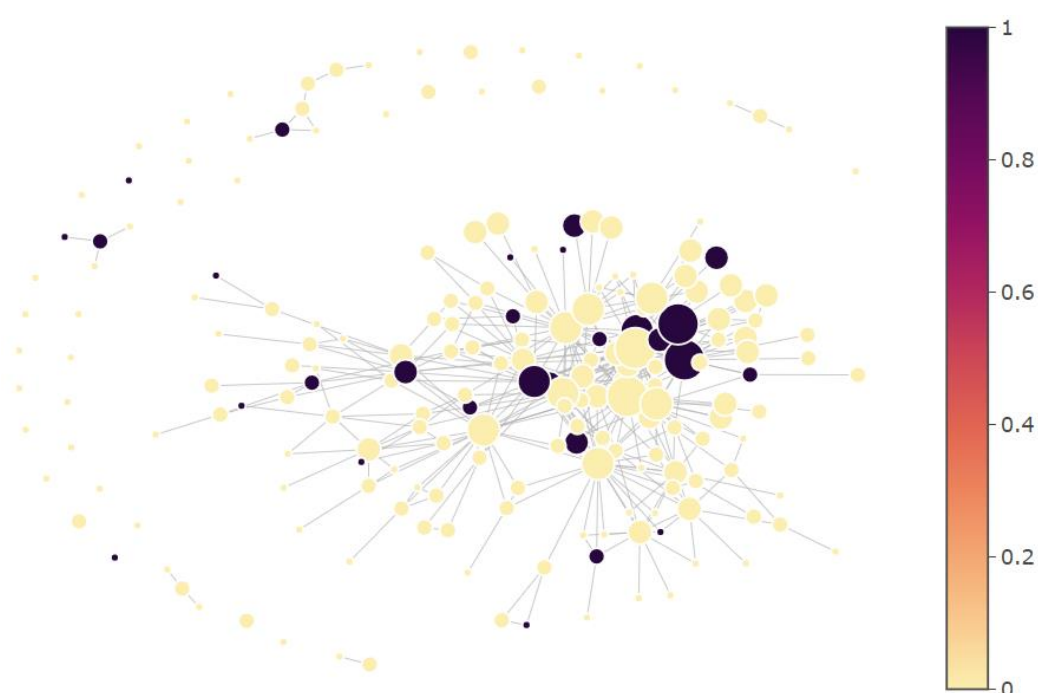


Figure S13. Topological data analysis of drugs in terms of drug classes. The nodes are clusters of drugs and the color indicates the distribution of drug classes. **a** Drug clustering vs. distribution of drugs in Benzenoids class (149 drugs included). **b** Drug clustering vs. distribution of drugs in Nucleosides, nucleotides, and analogues class (9 drugs included). **c** Drug clustering vs. distribution of drugs belonging to AHFS code 28:00:00 (136 drugs included).

d Drug clustering vs. distribution of drugs belonging to AHFS code 24:00:00 (72 drugs included).