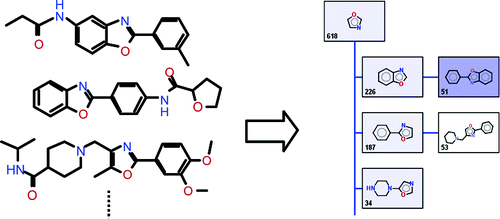
**The Scaffold Tree − Visualization of the Scaffold Universe by Hierarchical Scaffold Classification**

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## Abstract



A hierarchical classification of chemical scaffolds (molecular framework, which is obtained by pruning all terminal side chains) has been introduced. The molecular frameworks form the leaf nodes in the hierarchy trees. By an iterative removal of rings, scaffolds forming the higher levels in the hierarchy tree are obtained. Prioritization rules ensure that less characteristic, peripheral rings are removed first. All scaffolds in the hierarchy tree are well-defined chemical entities making the classification chemically intuitive. The classification is deterministic, data-set-independent, and scales linearly with the number of compounds included in the data set. The application of the classification is demonstrated on two data sets extracted from the PubChem database, namely, pyruvate kinase binders and a collection of pesticides. The examples shown demonstrate that the classification procedure handles robustly synthetic structures and natural products.

# Scaffold network generator: a tool for mining molecular structures

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## Abstract

**Summary:**Scaffold network generator (SNG) is an open-source command-line utility that computes the hierarchical network of scaffolds that define a large set of input molecules. Scaffold networks are useful for visualizing, analysing and understanding the chemical data that is increasingly available through large public repositories like PubChem. For example, some groups have used scaffold networks to identify missed-actives in high-throughput screens of small molecules with bioassays. Substantially improving on existing software, SNG is robust enough to work on millions of molecules at a time with a simple command-line interface.

**Availability and implementation:**SNG is accessible at <http://swami.wustl.edu/sng>

# ScaffoldGraph: an open-source library for the generation and analysis of molecular scaffold networks and scaffold trees

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**Summary**

ScaffoldGraph (SG) is an open-source Python library and command-line tool for the generation and analysis of molecular scaffold networks and trees, with the capability of processing large sets of input molecules. With the increase in high-throughput screening data, scaffold graphs have proven useful for the navigation and analysis of chemical space, being used for visualization, clustering, scaffold-diversity analysis and active-series identification. Built on RDKit and NetworkX, SG integrates scaffold graph analysis into the growing scientific/cheminformatics Python stack, increasing the flexibility and extendibility of the tool compared to existing software.

**Availability and implementation**

SG is freely available and released under the MIT licence at

<https://github.com/UCLCheminformatics/ScaffoldGraph>.