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Assignment Sheet 5

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A.5.1: Murcko Scaffold: Part I

In their paper, Bemis and Murcko suggest to organize structural data of atom groups into different types such as ring,linker, frameworks that proved to be quite effective in order to identify certain patterns in molecules. Especially some frameworks occur in almost half of the drugs in the database. Therefore it shows a low diversity of shapes in the set of known drugs. The diversity of the scaffolds is one of many key aspects to characterize compound screening libraries.[1]
When the molecules are represented using atomic and graph properties, an archetype for each instance can be considered and used to analyze hierarchy of the molecule from top to bottom.
For this the molecule is split into four units: ring systems, linker atoms, side chain atoms and frameworks Frameworks are emphasized when it comes to new drug discovery. Each atom bonded to another one is seen as side chain and gets removed until each atom is bonded to at least two other atoms. Then atoms that are rings are identified. Any atom not part of the ring is a linker atom the obtained result is the framework. [2] The characterization workflow is shown in Figure 1

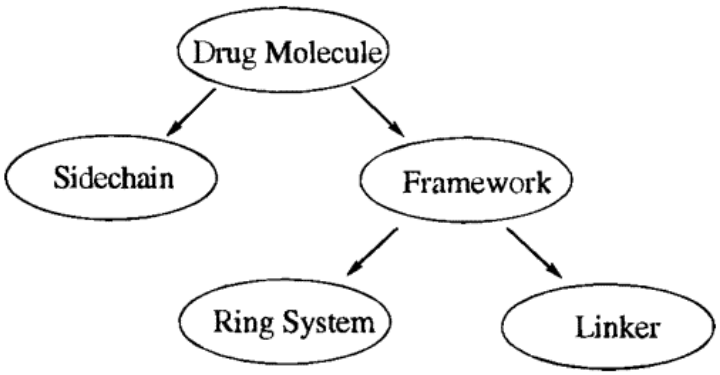

Figure 1: Hierarchical description of molecules.

[1] https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3180201/
[2] https://pubs.acs.org/doi/10.1021/jm9602928

A.5.2: Murcko Scaffold: Part II

The frameworks of the structures are marked in red. Side chains got removed leaving only linkers and the ring systems behind. Therefore the whole third structure is not seen as a proper molecule and gets removed completely due to the missing ring system.

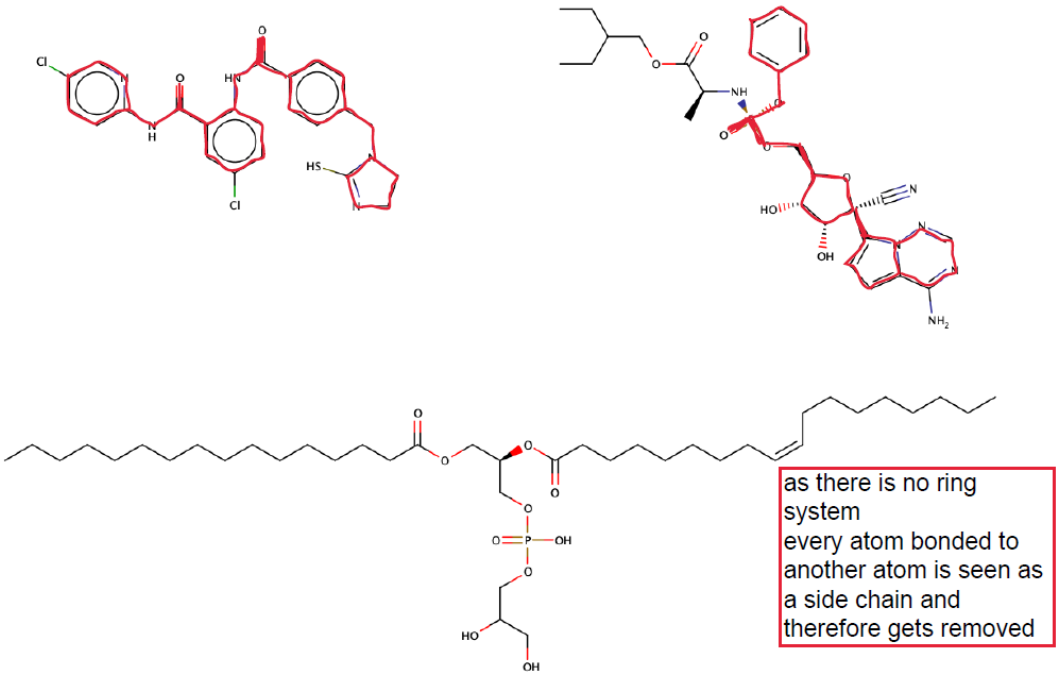

Figure 2: Frameworks of the provided structures.