Drug structural analysis

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Drug likeness analysis is widely used in modern drug design. However, most drug likeness filters, represented by Lipinski's "Rule of 5", are based on drug's simple structural characteristics (such as molecular number of hydrogen bond donors and acceptors) and physiochemical properties (such as ClogP). In this study, we conducted a thoroughly structural analysis for a set of 6515 know drugs. For each drug molecule, all possible fragments were enumerated by a brutal force approach. Those drug skeletons and fragments extensively used by drugs were identified. The drug likeness of those skeletons and fragments was further assessed by comparing the occurrence frequencies in the drug data set (6515 entries) and in a screening data set (1.95 million entries). The results obtained in this study could provide useful hints to medicinal chemists to design drug-like compounds as well as broaden the definition of drug-likeness of molecules.