Over the past decade, the attrition rate of clinical trials in drug discovery reached 90%. Although these approaches can rapidly filter out drug-like compounds, simple boundaries for individual physicochemical properties are too strict. Since then, a variety of relevant drug-likeness rules based on simple molecular properties have been developed, such as those proposed by Ghose et al. [9], Oprea et al. [10], Veber et al. [11], and Muegge et al. [12]. Pharmaceutical companies spend millions of dollars to advance a new drug through clinical trials and, thus, failure in the later stages of drug development typically result in significant economic losses [3]. Therefore, selecting appropriate candidates with a good balance of potency along with absorption, distribution, metabolism, excretion, and toxicity (ADMET) is an urgent scientific need. Undesirable PK properties and unacceptable toxicity are the main causes of the failure of drug candidates at the clinical trial stage [4]. These rules suggest that compounds that fall within a particular range are 'drug-like'.