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A systematic analysis of physicochemical and ADME properties of kinase inhibitors approved by US FDA prior to 2016

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In today's fast-paced and competitive environment, there is an ever-increasing need for more effective and efficient drug design by fully balancing potency, selectivity, molecular properties and appropriate ADME properties early in drug discovery. However, incorporating drug-like properties at the onset is often challenging. Understanding the physicochemical and ADME properties of successful drugs may provide helpful insight in better defining optimization parameters to facilitate this process. We compiled physicochemical and ADME data on kinase inhibitors

approved before 2016 and performed a systematic analysis of the common physicochemical and ADME features of these marketed drugs. Although the dataset is limited, valuable conclusions were drawn, which we believe are helpful in selecting helpful assays in a stage-appropriate manner and setting up optimization and advancement criteria during the discovery process. Just as crucial, this work can eliminate unnecessary studies. Details of this work will be presented.

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