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The Potential of One-Shot Learning for Drug Discovery – A Review

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Compounds with specific chemical properties for the treatment of diseases are sought out through drug discovery. The search for drugs can be made more efficient, less expensive, and less time-consuming by incorporating automation. New approaches and technologies in drug discovery have grown dramatically over the past few decades. "One-shot" learning is the best hope for the widespread adoption of machine learning in all industries. In this study, the authors show how one-shot learning can reduce the amount of data required to make meaningful predictions in drug discovery applications. With Few-Shot Learning (also referred to as One-Shot Learning), models can be trained to learn the desired goal with less data, like how humans do it. The objectives of the study are to explore the most prominent ways to identify and forecast drug discovery, potential applications as well as several of the remaining challenges. Chemical structures can be represented using some structural descriptors, a similarity measure is used to compare them, and a strategy can be used to predict the activity of a query compound in this manner. We expect this review to serve as an impetus for future experiments that seek to validate the use of one-shot learning in the chemical sciences.

Keywords: *one-shot learning, few-shot learning, drug discovery, machine learning*