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Artificial intelligence in the early stages of drug discovery

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Abstract

Although the use of computational methods within the pharmaceutical industry is well established, there is an urgent need for new approaches that can improve and optimize the pipeline of drug discovery and development. In spite of the fact that there is no unique solution for this need for innovation, there has recently been a strong interest in the use of Artificial Intelligence for this purpose. As a matter of fact, not only there have been major contributions from the scientific community in this respect, but there has also been a growing partnership between the pharmaceutical industry and Artificial Intelligence companies. Beyond these contributions and efforts there is an underlying question, which we intend to discuss in this review: can the intrinsic difficulties within the

drug discovery process be overcome with the implementation of Artificial Intelligence? While this is an open question, in this work we will focus on the advantages that these algorithms provide over the traditional methods in the context of early drug discovery.

Keywords: Artificial Intelligence; Deep learning; Drug discovery; Hit and lead identification; Machine learning; Property prediction; Target identification.

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