Chapter 17
Enhancing Pharmaceutics With AI Through Predictive Modeling of Crystal Structures and Atom Properties for Improved Solubility and Bioavailability

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ABSTRACT

The research study explores how sophisticated machine learning algorithms, i.e., our suggested model SENET, coupled with SVM and ADAM, could enhance drug solubility and bioavailability through the prediction of crystallographic structures

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and atom property classification. The current research aims to revolutionize pharmaceutical drug development processes by embracing AI-based preclinical Testing. We investigate the sophisticated field of crystallographic structures and dissect atomistic data in depth to reveal determining factors influencing crystal forms. The aim of the research is to enhance drug solubility and bioavailability by conducting this study, which will significantly transform pharmaceutical practice. The study shows that sophisticated machine learning methods can potentially forecast drug behavior in complicated situations. This study discloses the potential for groundbreaking drug discovery by speeding up the progress in pharmaceutical science, reducing the development cost, and optimizing patient benefit through enhanced drug delivery and action.

INTRODUCTION

One of the most significant predictive determinants of properties and behaviors of pharmaceutical drugs with a significant impact on their dimensions of solubility and bioavailability is crystallographic structures. The stability and dissolution rate of a drug and its overall efficacy will be reliant on the coordination of atoms in their crystalline state and, to a large extent, deterred by the complexities surrounding them. Understanding the complexities of crystallographic structures has been a daunting challenge in pharmaceutical science, largely due to the emphasis placed on these parameters. We address the complexity of crystallography using advanced machine learning algorithms, including not only our induced SENET model but also SVM and ADAM algorithms, to decode the specific details and order in these atomic structures while ensuring that crystal structures have careful atomistic data and that the factors influencing crystal geometries are at the level required. We are hoping that through deeper levels of scrutiny, we will overcome these traditional boundaries and reach new horizons that will predict drug solubility and bioavailability. We are not only researching to enhance our knowledge of pharmaceutical practice but also, hopefully, preparing the ground for new drug discovery that will, in the end, contribute to progress in pharmaceutical science and direct benefits such as reduced costs in drug development, as well as improved health outcomes for patients through improved delivery of the drug and its efficacy.

In an efficient manner, researchers propose a new methodology called Quick-CSP to predict crystal structures of similarly structured molecules in an effective manner. The methodology relies on valid and transferable custom-designed force fields and is also computationally less expensive Mattei, A., et al., 2022). . Crystal formation and crystal structure criteria are important to consider when developing a drug delivery system. Understanding the parameters in crystal formation and

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