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effective molecular representation learning is of great importance to facilitate molecular property prediction recent advances for molecular representation learning have shown great promise we present here some of the most popular electronic molecular and macromolecular representations used in drug discovery many of which are based on graph representations furthermore we describe applications of these representations in ai driven drug discovery effective representation of molecules is a crucial factor affecting the performance of artificial intelligence models this study introduces a flexible fragment based multiscale molecular it contains an introduction to the principles of gdl as well as relevant molecular representations such as molecular graphs grids surfaces and strings and their respective properties we first introduce molecular representation and property prediction methods and highlight newly emerging dl methods such as ensemble learning and transfer learning which have been used to solve some common problems in molecular representation in this paper we propose a representation learning method for molecular graphs called relmole which is featured by a hierarchical graph modeling of molecules and a contrastive learning scheme based on two level graph similarities molecular representation learning is an essential component of many molecule oriented tasks such as molecular property prediction and molecule generation in recent years graph neural networks gnns have shown great promise in this area representing a molecule as a graph composed of nodes and edges molecular modeling molecules neural networks abstract the accurate modeling and prediction of small molecule properties and bioactivities depend on the critical choice of molecular representation we present here some of the most popular electronic molecular and macromolecular representations used in drug discovery many of which are based on graph representations furthermore we describe applications of these representations in ai driven drug discovery a molecular representation is a representation of a molecule that can be read and processed by computers in order to use deep learning methods and acquire accurate molecular property prediction results it is necessary to find an appropriate molecular representation molecular representation learning mrl is a key step to build the connection between machine learning and chemical science in particular it encodes molecules as numerical vectors preserving the molecular structures and features on top of which the downstream tasks e g property prediction can be performed a molecular representation also known as descriptor of feature vectors encodes chemical identity of a molecular entity in terms of its chemical composition and atomic configuration only after the chemical identity is converted into a descriptor an array of numbers computer can efficiently process a large number of structures functional group representations e g a molecular access system maccs key fingerprint simply count the number of expert defined substructures present in a molecule and have a long history in the development of group additivity relationships simplified molecular input line entry system smiles is a text representation of molecules in a single line as it is sequential and composed of text methods inspired by nlp such as since a molecular graph is a natural representation of a molecule and conveys topological information several research in recent years have embraced it as a means of molecular representation gg nn 5 dmpnn 6 and deepatomiccharge 26 employed a message passing strategy for

molecular property prediction the ability to learn key patterns from complex sets of observations is a central intelligence 1 aspect of human expert chemists leverage this ability to find small molecule leads and optimize drug like properties in therapeutic discovery 2where intricate chemical and biological processes govern the interactions of small molecules understanding how to best represent molecules in a machine readable format is a key challenge 1 introduction representing chemical data in a concise and unambiguous way understandable by both humans and machines is not an easy task this is particularly true for the representation of molecules molecular geometry is the three dimensional arrangement of the atoms that constitute a molecule it includes the general shape of the molecule as well as bond lengths bond angles torsional angles and any other geometrical parameters that determine the position of each atom covalent molecules and compounds just as an atom is the simplest unit that has the fundamental chemical properties of an element a molecule is the simplest unit that has the fundamental chemical properties of a covalent compound some pure elements exist as covalent molecules the application of machine learning for chemical applications requires the conversion of molecular structures to a machine readable format known as a molecular representation the choice of

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of molecules and a contrastive learning scheme based on two level graph similarities

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