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speaking molecules can be represented in a machine readable format in four ways as a string with a connection table as a collection of features for example a fingerprint or series of physical descriptors or most recently with a computer learned representation using machine learning ml 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 1 introduction molecular representations underpin predictive generative and analytical tasks in drug discovery 1 the choice of a suitable representation can drastically impact the efficiency of discovering a novel drug candidate published 05 january 2024 enhancing geometric representations for molecules with equivariant vector scalar interactive message passing yusong wang tong wang shaoning li xinheng he mingyu a conceptual framework of molecular representation this post describes some codes used in the implementation of the above conceptual framework including reading drawing analyzing a molecule generating molecular fingerprint from a smiles string generating one hot encoding from a smiles string in this work we aim to leverage the representational power of a pretrained language model chemberta 2 20 by fusing the language representation to graph representations during fine tuning on the task of molecular property prediction published 17 february 2021 could graph neural networks learn better molecular representation for drug discovery a comparison study of descriptor based and graph based models dejun jiang zhenxing wu chang yu hsieh guangyong chen ben liao zhe wang chao shen dongsheng cao jian wu tingjun hou both the ball and stick model part c in figure 5 8 4 and the perspective drawing part d in figure 5 8 4 show the three dimensional structure of the molecule the latter also called a wedge and dash representation is the easiest way to sketch the structure of a molecule in three dimensions molecular representation learning with language models and domain relevant auxiliary tasks benedek fabian thomas edlich héléna gaspar marwin segler joshua meyers marco fiscato mohamed ahmed we apply a transformer architecture specifically bert to learn flexible and high quality molecular representations for drug discovery problems doi 10 1186 s13059 024 03273 z scientists at la jolla institute for immunology lji have developed a new computational method for linking molecular marks on our dna to gene activity their work

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