

Features/Descriptors

• Enable semantic input into machine learning models

- How would you describe a chemical in numbers that can be put into a mathematical formula?

- Features can be
 - from enumerable properties, e.g. number of a certain element, number of H bond donors/acceptors, presence/absence of an element functional group
 - based on 3D structures
 - of a chemical, e.g. surface area, radius of gyration, moments of inertia
 - of a protein-ligand complex

- <http://www.rdkit.org/docs/GettingStartedInPython.html#list-of-available-descriptors>



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Algorithms