

Basically, molar or weight scales are typical representations of the properties measured for molecular ensembles (substances). This was recently extended by the so called single molecule biology. Here we compare a large property datasets including biological activity (ChEMBL, PubChem) analyzing their relation to the aforementioned representations. The question of the maximal potency of ligands inspired the development and application of ligand efficiency (LE) estimators in drug design. LE which is a ratio of IC<sub>50</sub> to heavy atom counts (HAC) could be interpreted as a property representation type. Most often LE is analyzed as a function of HAC. Here LE is compared to the series of other properties of chemical compounds typically measured in the molar or weight scales. In the drug design literature LE has appeared controversial. This inspired the development of the new estimators: PLE, pPLE and SCORE which was described and analyzed in this work.

LE could also be interpreted in a single molecule scale, defining a potency of a single HAC This represents a molecular fragmentation. The dual representation of chemical compounds by molecules and substances decides that uncertainty of such fragmentation. This uncertainty can be described by a paradox similar to the Zenon paradox referring to the uncertainty of the division of space and time .