Abstract

Structure-activity relationship is an essential concept in chemistry guiding, for example, drug design. However, we need economics to fully understand the fate of drugs on the market. Quantitative structure-economy relationships (QSER) for a large dataset of a commercial building block library of over 2.2 million chemicals have been modeled and analyzed for the first time. Our study shows how data binning could be used as an informative method when analyzing big data in chemistry. The modeled molecular statistics shows that on average what we are paying for is the quantity of matter. The influence of synthetic availability scores is also revealed. Finally, we are buying substances by looking at the molecular graphs or molecular formulas. Thus, those molecules that have a higher number of atoms look more attractive and are, on average, also more expensive.