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# Unlocking stereochemical diversity

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A little more than 50 years ago Pfeiffer [1] noted that the more active a chiral drug was, the less active its enantiomer was. Recent years have seen increased success in screening compounds *in silico*. While the majority of 2D screening approaches are insensitive to stereochemistry, this is not the case in 3D docking, which is typically used to refine compound lists. Unfortunately, a number of common workflows result in generation of only one member of the number of structures actually registered in a 2D database [2]. This results in a fraction of candidate structures being ignored *in silico*, even though they are present in the real compound libraries being considered.

How big is the omitted chemistry space? What fraction of compounds in common databases are racemic mixtures, and how common are diastereomers and meso-compounds?

We will present workflows using KNIME to explore some of these questions, to properly enumerate specific stereoisomers present in molecular collections and to qualify the effects of enumeration on 3D compound screening.

## References

1. Pfeiffer CC: *Science* 1956, **124:**29.
2. Brooks WH, Daniel KG, Sung S-S, Guida WC: *J Chem Inf Model* 2008, **48:**639.