

## **Abstract**

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### **On entropy-based molecular descriptors: Statistical analysis of real and synthetic chemical structures**

This paper presents an analysis of entropy-based molecular descriptors. Specifically, we use real chemical structures, as well as synthetic isomeric structures, and investigate properties of and among descriptors with respect to the used data set by a statistical analysis.

Our numerical results provide evidence that synthetic chemical structures are notably different to real chemical structures and, hence, should not be used to investigate molecular descriptors. Instead, an analysis based on real chemical structures is favorable.

Further, we find strong hints that molecular descriptors can be partitioned into distinct classes capturing complementary information.