

## **Computational Chemistry and Artificial Intelligence**

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Computational chemistry is a broad field that uses computer simulations to help solving chemical problems. The computational results normally complement the information obtained from chemical experiments and in some cases provide unobserved chemical properties. However, today there are parts of the chemistry in which experiments are much faster than calculations, thus reducing the applications and the value of computational methods. Fortunately, the rapid explosion of the field of artificial intelligence can help solve the problem of the speed of some computational approaches. The paper will present examples of application of machine learning in computational chemistry applied to pharmaceutical chemistry and drug design.