Quantum chemistry in Pharmaceutical Development at AstraZeneca

By

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Modeling and simulation has been one of the cornerstones in product development in many industries for many years. For instance computational fluid dynamics and finite element modeling have been utilized to guide design in the automotive industry since the early 1990ies. Similarly regression methods and statistical modeling have been embedded in the drug discovery phase of the drug hunting process. Regression methods relying on simple molecular descriptors have become widespread in this field. Some advances towards usage of more fundamental molecular descriptors derived from quantum chemical calculations in regression models have started to surface.
In the development phase fewer molecules are processed and more detailed models could be used. In this poster I will exemplify a few areas eg. using quantum chemistry to increase understanding of degradation reaction pathways of active compounds. In addition, I will describe the initiative AstraZeneca have devised to build up a modeling capability within our unit. We are currently focusing on extending our capability in modeling chemical reactivity and material design area.